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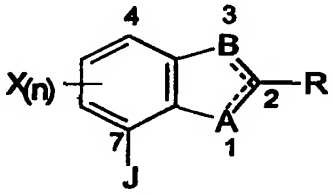
(54) Title: CYCLOIMIDO–SUBSTITUTED BENZOFUSED HETEROCYCLIC HERBICIDES

(57) Abstract



(I)

Novel herbicidal compounds, compositions containing them, and methods for their use in controlling weeds are disclosed. The novel herbicidal compounds are represented by formula (I), where J is a 1–substituted–6–trifluoromethyl–2,4–pyrimidinedione–3–yl, a 1–substituted–6–trifluoromethyl–1,3,5–triazine–2,4–dion–1–yl, a 3,4,5,6–tetrahydrophthalimid–1–yl, a 4–difluoromethyl–4,5–dihydro–3–methyl–1,2,4–triazol–5(1H)–on–1–yl, a 5,6,7,8–tetrahydro–1H,3H–[1,3,4]thiadiazolo[3,5–a]pyridazineimin–1–yl, or a 1,6,8–triazabicyclo[4.3.0]–nonane–7,9–dion–8–yl ring attached at the 7 position of a benzofuran, benzoxazole, indole, 2,3–dihydrobenzimidazole or benzimidazole, and X is selected from hydrogen, halogen, cyano, nitro, and amino. Preferred R groups are optionally substituted alkyl groups.

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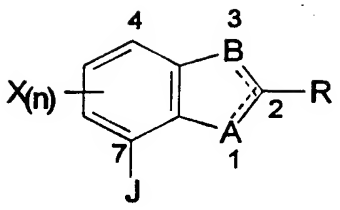
CYCLOIMIDO-SUBSTITUTED BENZOFUSED HETEROCYCLIC HERBICIDES

BACKGROUND OF THE INVENTION

The present invention relates generally to novel herbicidal compounds and methods for their use in controlling unwanted plant species in agriculture. In particular, the present invention pertains to cycloimido-substituted benzofused heterocyclic herbicides, and more particularly it pertains to herbicides in which the benzofused heterocycle is a benzofuran, benzimidazole, a 2,3-dihydrobenzimidazole, or indole having a cycloimido moiety which is a 1-substituted-6-trifluoromethyl-2,4-pyrimidinedione-3-yl, a 1-substituted-6-trifluoromethyl-1,3,5-triazine-2,4-dion-1-yl, a 3,4,5,6-tetrahydrophthalimid-1-yl, a 4-difluoromethyl-4,5-dihydro-3-methyl-1,2,4-triazol-5(1H)-on-1-yl, a 5,6,7,8-tetrahydro-1H,3H-[1,3,4]thiadiazolo[3,5-a]pyridazineimin-1-yl, or a 1,6,8-triazabicyclo[4.3.0]-nonane-7,9-dion-8-yl ring.

SUMMARY OF THE INVENTION

It has now been found that certain cycloimido-substituted benzofused heterocyclic compounds are useful as pre-emergent and postemergent herbicides. These novel compounds are represented by formula **I:**

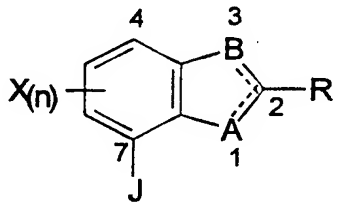


I

where J is a 1-substituted-6-trifluoromethyl-2,4-pyrimidinedione-3-yl, a 1-substituted-6-trifluoromethyl-1,3,5-triazine-2,4-dion-1-yl, a 3,4,5,6-tetrahydrophthalimid-1-yl, a 4-difluoromethyl-4,5-dihydro-3-methyl-1,2,4-triazol-5(1H)-on-1-yl, a 5,6,7,8-tetrahydro-1H,3H-[1,3,4]thiadiazolo[3,5-a]pyridazineimin-1-yl, or a 1,6,8-triazabicyclo[4.3.0]-nonane-7,9-dion-8-yl ring attached at the 7 position of a benzofuran, benzoxazole, 2,3-dihydrobenzimidazole, indole or benzimidazole, and X is selected from hydrogen, halogen, cyano, nitro, alkyl, haloalkyl, and amino. Preferred R groups are optionally substituted alkyl groups.

DETAILED DESCRIPTION OF THE INVENTION

Certain cycloimido-substituted benzofused heterocyclic compounds have now been found to be useful as pre- and postemergent herbicides. These compounds are represented by formula I:



I

where

(1) A is nitrogen double-bonded to position 2 and B is oxygen;

(2) A is oxygen and B is CR^1 double bonded to position 2;

(3) A is NH and B is nitrogen double-bonded to position 2;

(4) A is nitrogen double bonded to position 2 and B is NR^2;

(5) A is CH double bonded to position 2 and B is NR^2;

(6) A is NH and B is CR^1 double bonded to position 2; or

(7) A and B are NH

R is hydrogen, hydroxy, mercapto, straight or branched chain lower alkyl, cycloalkyl, alkoxy, aryl, heteroaryl, alkenyl, haloalkyl, hydroxyalkyl, haloaryl, alkoxyaryl, arylalkyl, aryloxyalkyl, haloarylalkyl, alkylthio, heterocyclyl, alkoxyalkyl, alkoxylalkyloxyalkyl, alkylcarbonyloxyalkyl, arylcarbonyloxyalkyl, aminocarbonyloxyalkyl, aminoalkyl, cyanoalkyl, aminoalkenyl, carboxy, carboxyalkyl, alkylcarboxy, alkylcarboxyalkyl, formyl, aminocarbonyl, amino, oxygen, cyano, nitro, alkylsulfonyl, aminosulfonyl, alkylsulfonylamino, alkoxycarbonyloxyalkyl, alkylcarboxylalkoxy, alkoxycarbonylamino, alkoxycarbonylalkylaminoalkyl, aryliminoalkyl, (aryl)(alkoxy)alkyl, (aryl)(alkylcarbonyloxy)alkyl, arylalkoxyalkyl, cyanoalkylthio, alkynylalkylthio, arylalkylthio, cyanothio, cyanothioalkyl, alkoxycarbonylalkylthio, aminocarbonylalkylthio, alkenylalkylthio, haloalkylalkynylalkylthio, aminocarbonyloxyalkyl, arylalkylcarbonylaminoalkyl, (hydroxy)(aryl)alkyl, alkylcarbonylaminoalkyl, alkylsulfonylaminoalkyl, aminocarbonylalkyl, alkoxycarbonyl, and alkenyloxy, where the amino group may be substituted with one or two substituents independently selected from alkyl, hydroxy, alkoxy, carboxy, aryl, alkylsufonyl, or haloalkylsulfonyl;

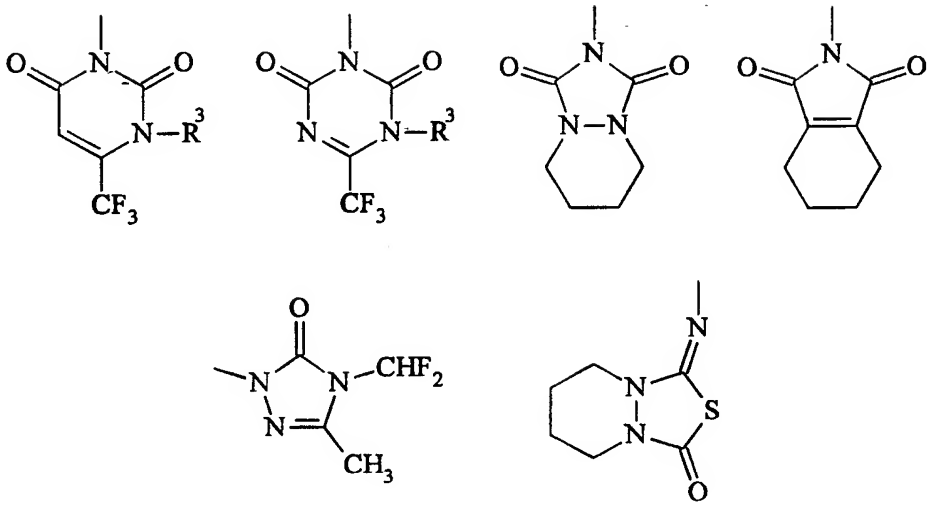
R^1 is hydrogen, lower alkyl, or haloalkyl;

R^2 is hydrogen, alkyl, haloalkyl, CO_2(alkyl), CH_2CO_2(alkyl), CH_2CONH-alkyl, $CH_2CON(alkyl)_2$, CH_2CO_2H, CH_2OCH_3, SO_2(alkyl), $CH_2CH{=}CH_2$, $CH_2C{\equiv}CH$.

X is selected from hydrogen, F, Cl, Br, alkyl, haloalkyl, CN, NO_2, and NH_2;

n is 0-3;

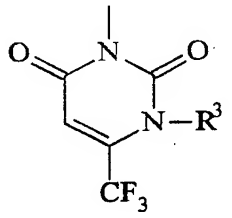
J is selected from



and

R^3 is selected from hydrogen, alkyl, haloalkyl, CH_2CN, $CH_2CH=CH_2$, $CH_2C\equiv CH$, CH_2CO_2(alkyl), CH_2OCH_3, and NH_2.

Preferred compounds are those of formula I where R is CH_3, CH_2CH_3, $C(CH_3)_2OH$, CH_2CH_2OH, $CH(CH_3)_2$, t-butyl, CF_3, $CH(F)CH_3$, CF_2CF_3, $C(CH_3)_2OCOCH_3$, $C(CH_3)_2NHSO_2CH_3$, $CH_2CH_2C\equiv N$, $CH_2CH_2CO_2CH_3$, and $CON(CH_3)_2$; X is a chlorine, bromine or fluorine substituted in one or both of positions 4 and 6; J is



and R^3 is CH_3 or NH_2.

One aspect of the present invention relates to compounds of formula I in which A is nitrogen double-bonded to position 2 and B is oxygen, and R, R^3, J, X and n are as described above.

Another aspect of the present invention relates to compounds of formula I in which A is oxygen and B is CR^1 double bonded to position 2, and R, R^1, R^3, J, X and n are as described above.

Another aspect of the present invention relates to compounds of formula I in which A is NH and B is nitrogen double-bonded to position 2, and R, J, X and n are as described above.

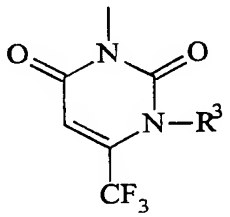
Another aspect of the present invention relates to compounds of formula I in which A is nitrogen double bonded to position 2 and B is NR^2,and R, R^2, R^3, J, X and n are as described above.

Another aspect of the present invention relates to compounds of formula I in which A is CH double bonded to position 2 and B is NR^2, and R, R^2, R^3, J, X and n are as described above.

Another aspect of the present invention relates to compounds of formula I in which A is NH and B is CR^1 double bonded to position 2, and R, R^1, R^3, J, X and n are as described above.

Another aspect of the present invention relates to compounds of formula I in which A and B are NH and R, R^1, R^3, J, X and n are as described above.

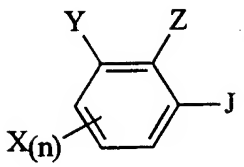
Another aspect of the present invention relates to compounds of formula I where J is not



when: A is oxygen and B is CR^1 double bonded to position 2; A is CH double bonded to position 2 and B is NR^2; or A is NH and B is CR^1 double bonded to position 2; and R, R^1, R^3, X, and n are as described above.

As shown in the specification a wide range of substituents is described for position B in compounds of formula I whereas position A is generally unsubstituted. It was found that some herbicidal activity is retained when a methyl substituent is placed at position A, but that substitution at that position generally causes a sharp decrease in activity.

Certain intermediates of the present invention are novel. These include compounds of formula II:

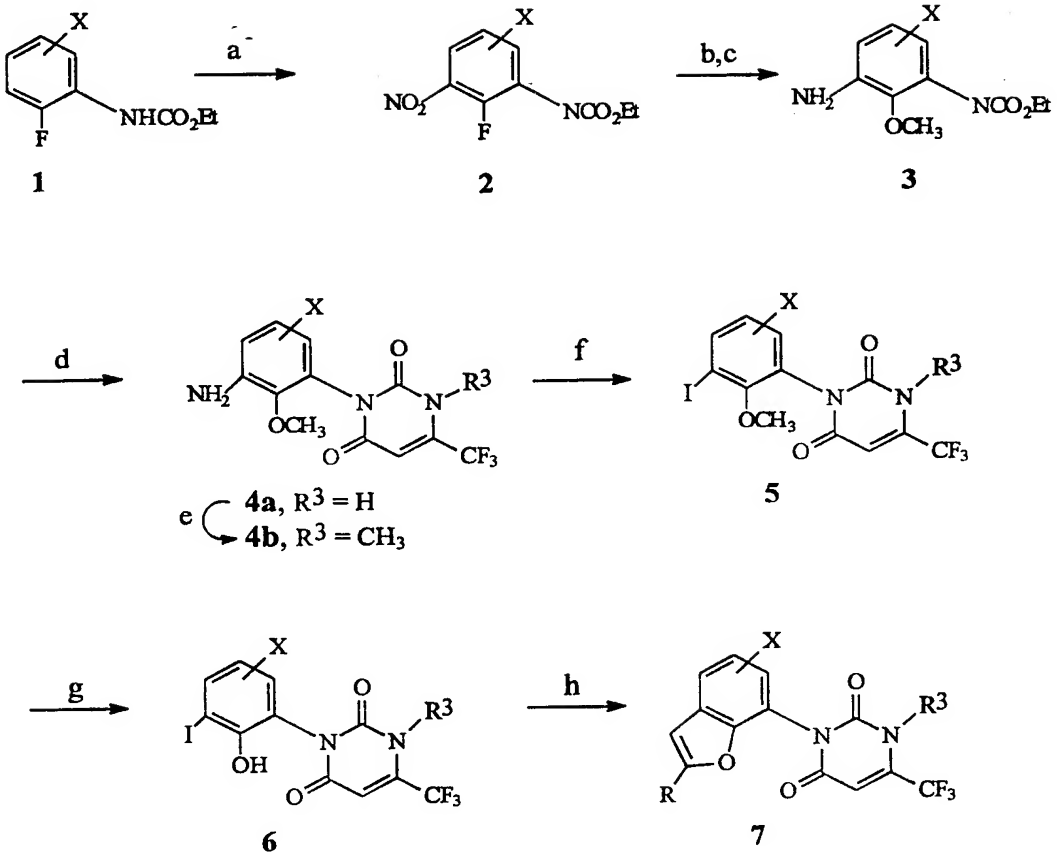


II

where Y is NO_2, NH_2, or -NHN=C(CH_3)R; Z is hydrogen, F, NH_2 or OH; and R, J, X, and n are as described above; with the proviso that when Y is -NHN=C(CH_3)R, Z is hydrogen.

As used in this specification and unless otherwise indicated, the terms "alkyl," "alkenyl," "alkynyl," "haloalkyl," and "alkoxy" used alone or as part of a larger moiety, includes straight or branched carbon chains of 1 to 6 carbon atoms. "Halogen" refers to fluorine, bromine or chlorine. "THF" means tetrahydrofuran, "DMF" means N,N-dimethylformamide, and "DBU" means 1,8-diazabicyclo[5.4.0]undec-7-ene. When "n" in "$X_{(n)}$" is 2 or 3, the substituents X may be the same or different from one another.

Scheme 1

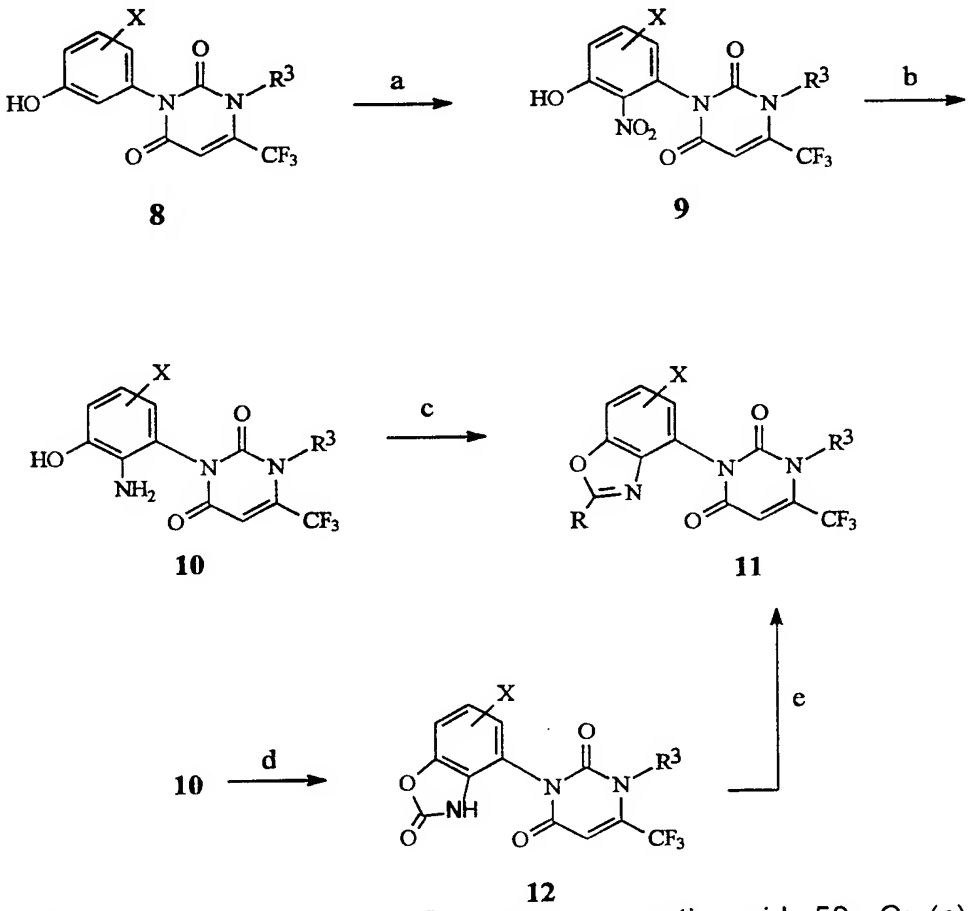


a) 70% HNO_3/H_2SO_4, 0-5 ∘C; (b) $NaOSi(CH_3)_3$, MeOH, dioxane; (c) Fe, EtOH, acetic acid, HCl, heat; (d) $CF_3C(NH_2)=CO_2CH_2CH_5$, $NaOSi(CH_3)_3$, DBU, DMF; (e) CH_3I, K_2CO_3, DMF, 60-80 °C; (f) HCl, $NaNO_2$ NaI, H_2O; (g) BBr_3 CH_2Cl_2 (h) HC≡CR, $Pd(Ph_3P)_2Cl_2$, CuI, triethylamine.

Benzofurans of formula **I**, where A is oxygen and B is CH double bonded to position 2, may be generally prepared as shown in Scheme 1. Starting with an appropriately substituted fluoroaniline derivative **1**, nitration provides intermediate **2**. Displacement of the fluorine of **2** with a methoxy group as shown in step b, followed by reduction of the nitro group as shown in step c provide the methoxyaniline **3**. The methoxyaniline **3** is a versatile intermediate from which a number of compounds of the present invention can be made by attachment of various J groups. For example, a uracil ring may be appended as shown in step d to give intermediate **4a**. At this point, R^3 substituents other than H may be introduced, as shown for example in step e to provide **4b** where R^3 is methyl.

Using diazotization conditions (step f) **4b** is converted to the iodoanisole **5** which is then deprotected to give the iodophenol **6**. Palladium-catalyzed acetylenic coupling and ring closure as shown in step h give benzofurans **7** of the present invention. To obtain benzofurans of formula **I** where the J group is other than uracil, approaches analogous to that outlined in Scheme 1 may be followed. Such approaches based on Scheme 1 would be known to one skilled in the art.

Scheme 2

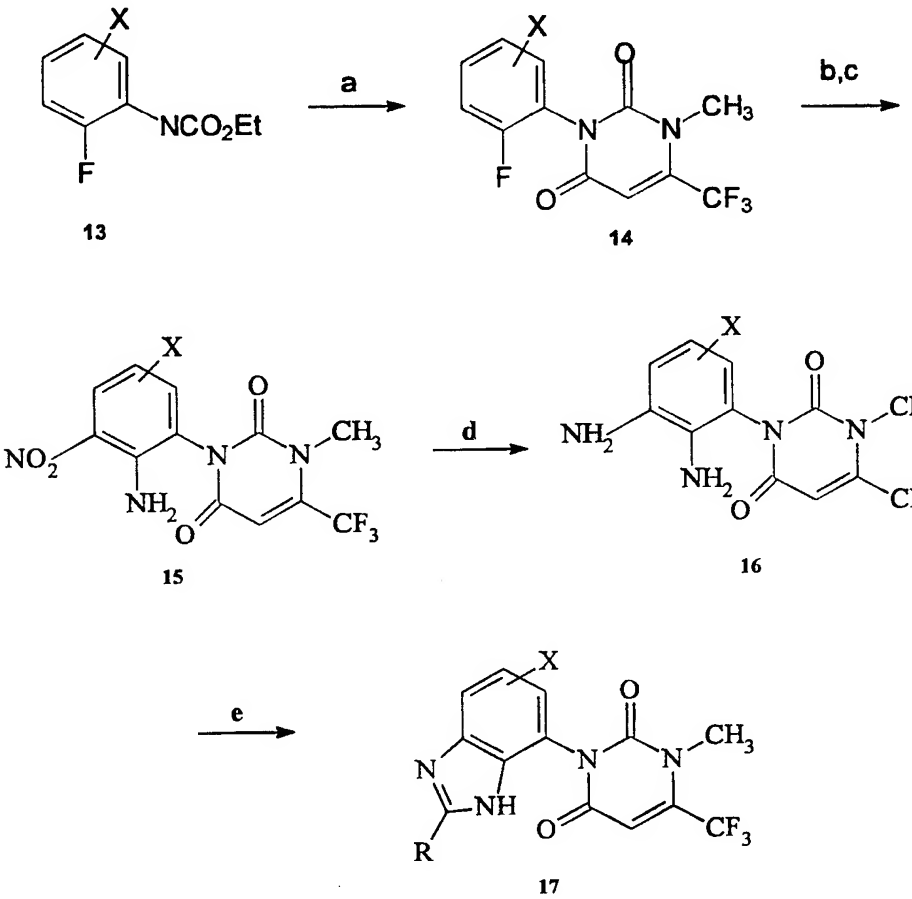


a) 70% HNO_3/H_2SO_4 0-5 ◦C; (b) Fe, aqueous acetic acid, 50 ◦C; (c) RCOCl, pyridinium p-toluenesulfonate, triethylamine, xylene; (d) 1,1-carbonylimidazole, THF; (e) R'-halide, Ag_2O, CH_2Cl_2 (to give **11** where R=R'O).

Benzoxazoles of formula I, where A is nitrogen double bonded to position 2 and B is oxygen, may be prepared as shown in Scheme 2 above. Starting with a phenol such as intermediate **8** nitration under standard conditions

gives the nitrophenol **9**. Certain of the benzoxazoles **11** of the present invention may be obtained by reduction of **9** to the aniline **10** followed by treatment with an acid halide (such as shown in step c). Alternatively, other benzoxazoles **11** may be obtained by treating **10** with carbonyldiimidazole to give intermediate **12** which can be O-alkyated according to step e. The approach outlined in Scheme 2 can be adapted, in ways known to one skilled in the art, to obtain benzoxazoles of formula **I** where the J group is other than uracil.

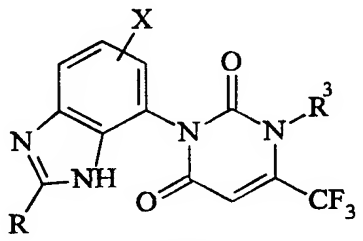
Scheme 3



a) see steps (d) and (e) of Scheme 1; (b) 70% HNO_3/H_2SO_4, 0-5 °C; (c) NH_4OAc, triethylamine, dioxane, heat; (d) $SnCl_2 \cdot H_2O$ or Fe, NH_4Cl, aqueous ethanol, heat; (e) RCO_2H, heat; RCO-halide, CH_2Cl_2/Pyridine, then $POCl_3$, CH_2Cl_2; alkoxycarbonyl isothiocyanate, $HgCl_2$, heat (where R is $-NHCO_2$alkyl); or thiophosgene, EtOAC, heat (where R is -SH).

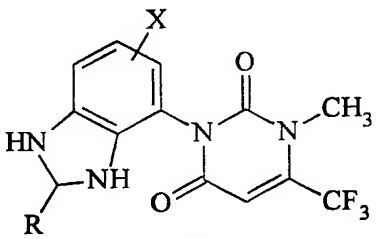
Benzimidazoles of formula I, where A is NH and B is nitrogen double bonded to position 2, may be prepared as shown in Scheme 3 above. For example,

intermediate **13** may be converted to the uracil **14** by the well-known chemistry previously described. Nitration of **14** followed by aminolysis of the fluorine group (steps b and c) provides the nitroaniline **15**. The diamine **16** is obtained by reduction of **15** under standard conditions. Benzimidazoles **17** of the present invention are obtained by treatment of **16** with a carboxylic acid, an acid halide, an alkoxycarbonyl isothiocyanate, or thiophosgene according to step e. Other benzimidazoles 17 of the present invention are obtained by derivativization of benzimidazoles depicted in Scheme 3 using techniques known to one skilled in the art. The approach outlined in Scheme 3 can be adapted, in ways known also to one skilled in the art, to obtain benzimidazoles of formula I where the J group is other than uracil.



17A

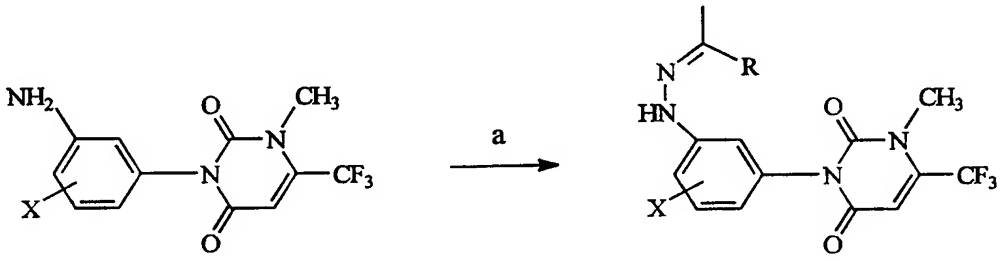
Benzimidazoles of structure 17A where R^3 is NH_2 are prepared in a manner analogous to that depicted in Scheme 3, except the NH_2 group is attached following nitration of the phenyl ring. The 1-unsubstituted uracil ring is formed as previously described in step d of Scheme 1, followed by nitration of the phenyl ring (Scheme 3, step b). The uracil ring is then aminated in the 1-position by methods known in the art by treating it with 1-aminooxysulfonyl-2,4,6-trimethylbenzene. The 1-aminouracil is then subjected to aminolysis of the phenyl fluorine (step c) followed by reduction to the diamine (step d).



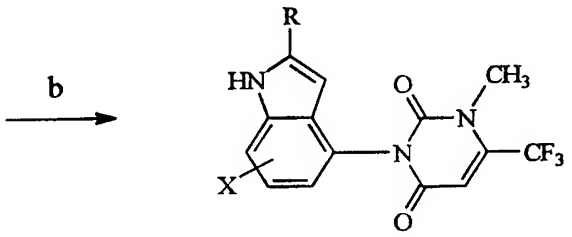
17B

2,3-Benzimidazoles of formula I, where A and B are NH may be prepared from Intermediate 16 in Scheme 3 by heating it with an appropriately substituted acetaldehyde ethyl hemiacetal, affording compounds of Structure 17B.

Scheme 4



18 **19**



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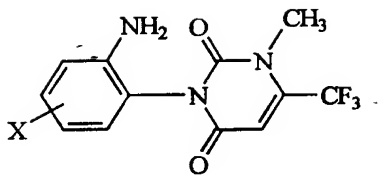
a) i. $NaNO_2$, HCl; ii. $SnCl_2 2H_2O$; iii. $RCOCH_3$; (b) polyphosphoric acid, 80 °C.

Indoles of formula I, where A is CH double bonded to position 2 and B is NR^1, may be prepared according to Scheme 4 above. Using a Fischer indole route the starting aniline **18** may be converted to the corresponding hydrazone **19** which in turn may be cyclized under acidic conditions such as is shown in step b. The resulting indoles **20** of the present invention may be further derivatized by alkylation of the indole ring nitrogen to indoles of formula I where R^1 is other than hydrogen. The approach outlined in Scheme 4 can be adapted, in ways known to one skilled in the art, to obtain indoles of formula I where the J group is other than uracil.



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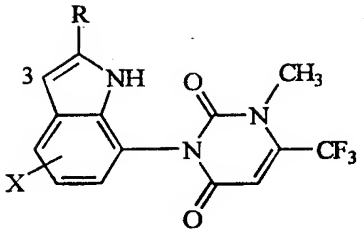

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Indoles of formula I, where A is NH and B is CR^1 double bonded to position 2, may be prepared by a Fischer indole synthesis analogous to that shown in Scheme 4 starting with aniline **21**. Substitution at the 3 position of indoles such as **22** with R^1 groups is known to one skilled in the art.

Compounds of the present invention may also be prepared in accordance with the procedures shown in the Examples below, by procedures analogous to those shown in the Examples, or by other methods that are generally known or available to one skilled in the art.

EXAMPLE 1

1-METHYL-6-TRIFLUOROMETHYL-3-[7-BROMO-5-FLUORO-2-(2-METHYLCARBONYLOXYPROP-2-YL)BENZOXAZOL-4-YL]-2,4(1H,3H)-PYRIMIDINEDIONE (COMPOUND 104)

Step A 1-methyl-6-trifluoromethyl-3-(4-bromo-2-fluoro-5-hydroxy-6-nitrophenyl)-2,4(1H,3H)-pyrimidinedione

A stirred solution of 17.0 grams (0.044 mole) of 1-methyl-6-trifluoromethyl-3-(4-bromo-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione and 5.0 grams (0.050 mole) of sulfuric acid in 100 mL of glacial acetic acid was cooled to 15 °C, and 3.2 grams (0.050 mole) of 70% nitric acid was added dropwise. The reaction mixture was then allowed to warm to ambient temperature where it stirred for two hours. The reaction mixture was poured into water and extracted with diethyl ether. The extract was concentrated under reduced pressure to a residue. The residue was purified by column chromatography on silica gel, yielding 16.4 grams of title compound; mp 76-78 °C.

Step B 1-methyl-6-trifluoromethyl-3-(6-amino-4-bromo-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione

A stirred solution of 16.0 grams (0.037 mole) of 1-methyl-6-trifluoromethyl-3-(4-bromo-2-fluoro-5-hydroxy-6-nitrophenyl)-2,4(1H,3H)-pyrimidinedione and 10 mL of water in 120 mL of glacial acetic acid was heated to 50 °C, and 16.0 grams (excess) of iron dust was slowly added. The reaction mixture was then cooled to ambient temperature where it stirred for one hour. The reaction mixture was filtered through diatomaceous earth, and the filtrate was partitioned in a mixture of 150 mL portions each of water and ethyl acetate. The organic layer was separated, dried with magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure to a residue. The residue was purified by column chromatography on silica gel, yielding 12.0 grams of title compound; mp 98-100 °C.

Step C Compound 104

A stirred solution of 0.50 gram (0.0013 mole) of 1-methyl-6-trifluoromethyl-3-(6-amino-4-bromo-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione, 0.21 gram (0.0013 mole) of 1-chlorocarbonyl-1-methylethyl acetate, 0.14 gram (0.0014 mole) of triethylamine, and 0.16 gram (0.0006 mole) of pyridinium p-toluenesulfonate in 50 mL of xylene was heated at 150 °C for about 18 hours. The reaction mixture was then cooled to ambient temperature and taken up in ethyl acetate. The solution was washed with water and an aqueous solution saturated with sodium chloride; then it was dried with magnesium sulfate. The mixture was filtered, and the filtrate was concentrated under reduced pressure to a residue. The residue was purified by column chromatography on silica gel, yielding 0.72 gram of Compound 104. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 2

1-METHYL-6-TRIFLUOROMETHYL-3-(7-BROMO-5-FLUORO-2-METHOXY-BENZOXAZOL-4-YL)-2,4(1H,3H)-PYRIMIDINEDIONE (COMPOUND 109)

Step A 1-methyl-6-trifluoromethyl-3-(7-bromo-5-fluorobenzoxazol-2-on-4-yl)-2,4(1H,3H)-pyrimidinedione

A stirred solution of 2.0 grams (0.005 mole) of 1-methyl-6-trifluoromethyl-3-(6-amino-4-bromo-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione and 1.2 grams (0.008 mole) of carbonylimidazole in 50 mL of **THF** was heated at reflux for three hours. The reaction mixture was cooled and concentrated under reduced pressure to a residue. The residue was purified by column chromatography on silica gel, yielding 1.1 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step B Compound 109

A mixture of 0.50 gram (0.001 mole) of 1-methyl-6-trifluoromethyl-3-(7-bromo-5-fluorobenzoxazol-2-on-4-yl)-2,4(1H,3H)-pyrimidinedione 0.17 gram (0.001 mole) of methyl iodode, and 0.27 gram (0.001 mole) of silver(I) oxide in 50 mL of methylene chloride was stirred at ambient temperature for two hours. The product was isolated from the reaction mixture by column chromatography on silica gel, yielding 0.28 gram of Compound 109. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 3

1-METHYL-6-TRIFLUOROMETHYL-3-[7-CHLORO-5-FLUORO-2-(1-METHYLETHYL)BENZOXAZOL-4-YL]-2,4(1H,3H)-PYRIMIDINEDIONE (COMPOUND 28)

Step A 1-methyl-6-trifluoromethyl-3-(4-chloro-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione

A stirred solution of 18.2 grams (0.054 mole) of 1-methyl-6-trifluoromethyl-3-(5-amino-4-chloro-2-fluorophenyl)-2,4(1H,3H)-pyrimidinedione in 100 mL of sulfuric acid was cooled to 5 °C, and a solution of 3.7 grams (0.054 mole) of sodium nitrite in about 10 mL of water was added dropwise. The reaction mixture was then warmed to ambient temperature where it stirred for two hours.

In a separate reaction vessel, a stirred mixture of 242 grams (0.970 mole) of copper(II) sulfate and 1.5 grams (0.005 mole) of iron(II) sulfate heptahydrate in about 300 mL of water and 300 mL of xylene was heated to reflux, and the pyrimidinedione diazonium solution prepared above was added dropwise. The reaction mixture was stirred at reflux for two additional hours, then allowed to cool as it stirred for about 18 hours. The reaction mixture was poured into about 600 mL of water, and the aqueous/organic layers were separated. The aqueous layer was washed with ethyl acetate, and the wash was combined with the organic layer. The combined organic material was washed with water, then with an aqueous solution saturated with sodium chloride. The organic material was dried with magnesium sulfate and filtered. The filtrate was concentrated under reduced pressure, yielding impure product. The product was dissolved in diethyl ether and washed with aqueous 10% hydrochloric acid, and with water. The diethyl ether solution was dried with magnesium sulfate and filtered. The filtrate was concentrated under reduced pressure, yielding 7.6 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step B 1-methyl-6-trifluoromethyl-3-(4-chloro-2-fluoro-5-hydroxy-6-nitrophenyl)-2,4(1H,3H)-pyrimidinedione

This compound was prepared in the manner of Step A of Example 1, using 3.8 grams (0.011 mole) of 1-methyl-6-trifluoromethyl-3-(4-chloro-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione, 1.0 gram (0.011 mole) of 70% nitric acid, and 50 mL of sulfuric acid, yielding 1.5 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step C 1-methyl-6-trifluoromethyl-3-(6-amino-4-chloro-2-fluoro-5-hydroxy-phenyl)-2,4(1H,3H)-pyrimidinedione

This compound was prepared in the manner of Step B of Example 1, using 1.5 grams (0.004 mole) 1-methyl-6-trifluoromethyl-3-(4-chloro-2-fluoro-5-hydroxy-6-nitrophenyl)-2,4(1H,3H)-pyrimidinedione, 3.0 grams (0.054 mole) of iron dust, and 5 mL of water in 50 mL of glacial acetic acid, yielding 1.0 gram of title compound. The NMR spectrum was consistent with the proposed structure.

Step D Compound 28

This compound was prepared in the manner of Step C of Example 1, using 0.52 gram (0.0015 mole) of 1-methyl-6-trifluoromethyl-3-(6-amino-4-chloro-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione, 0.18 gram (0.0017 mole) of isobutyryl chloride, 0.24 gram (0.0017 mole) of triethylamine, and 0.09 gram (0.0004 mole) of pyridinium p-toluenesulfonate in 50 mL of xylene, yielding 0.22 gram of Compound 28. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 4

SYNTHESIS OF 3-(4-CHLORO-6-FLUORO-2-PHENYLBENZOFURAN-7-YL)-1-METHYL-6-TRIFLUOROMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE (Compound 280)

Step A ethyl N-(4-chloro-2,6-difluoro-3-nitrophenyl)carbamate

A stirred solution of 23.6 grams (0.109 mole) of ethyl N-(4-chloro-2,6-difluorophenyl)carbamate in 125 mL of concentrated sulfuric acid was cooled to about 0 °C and 7.7 mL (0.123 mole) of 70% nitric acid was added dropwise at a rate to maintain the reaction temperature below 10 °C. Upon completion of addition, the reaction mixture was stirred at 10 °C for 30 minutes and then allowed to warm to ambient temperature where it stirred for about 18 hours. At the conclusion of this period, the reaction mixture was poured into 150 mL of ice-water. The resulting precipitate was collected by vacuum filtration and washed with water followed by petroleum ether. The precipitate was dried in a heated vacuum desicator, yielding 30.6 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step B ethyl N-(4-chloro-6-fluoro-2-methoxy-3-nitrophenyl)carbamate

Under a nitrogen atmosphere, a solution of 30.6 grams (0.109 mole) of ethyl N-(4-chloro-2,6-difluoro-3-nitrophenyl)carbamate and 18 mL (0.449 mole) of methanol in 175 mL of dioxane was stirred and 218 mL (0.218 mole) of 1M sodium trimethylsilanoate (in tetrahydrofuran) was added dropwise during a 45 minute period. Upon completion of addition, the reaction mixture was heated to 65 °C where it stirred for three hours. At the conclusion of this period, the reaction mixture was allowed to

cool to ambient temperature where it stirred for about 18 hours. The reaction mixture was concentrated under reduced pressure to a residue. The residue was taken up in cold 3N hydrochloric acid. The resulting solid was collected by filtration, washed with petroleum ether, and heat dried under vacuum, yielding 21.3 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step C ethyl N-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)carbamate

Under a nitrogen atmosphere, a stirred solution of 21.3 grams (0.072 mole) of ethyl N-(4-chloro-6-fluoro-2-methoxy-3-nitrophenyl)carbamate, 18.3 grams (0.328 mole) of iron powder, 50 mL of acetic acid, and 250 mL of ethanol was heated to 65° C where it stirred for two hours. At the conclusion of this time, 3 mL (0.036 mole) of 12M hydrochloric acid was added. Upon completion of addition, the reaction mixture was stirred for an additional two hours. After this time, the reaction mixture was concentrated under reduced pressure to yield a brown oil. The oil was then taken up in methylene chloride. The mixture was filtered through diatomaceous earth, and the filter cake was washed with water and an aqueous saturated sodium bicarbonate solution. The filtrate was stored over sodium sulfate for about 18 hours and then filtered. The solvent was removed under reduced pressure to yield a black oil. This oil was filtered through a silica gel pad, yielding 15.0 grams of ethyl N-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)carbamate. The NMR spectrum was consistent with the proposed structure.

Step D 3-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione

This compound was prepared using 4.0 grams (0.036 mole) of sodium trimethylsilanolate, 6.6 grams (0.036 mole) of ethyl 3-amino-4,4,4-trifluorocrotonate, 8.5 grams (0.032 mole) of ethyl N-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)carbamate, and 2.2 grams (0.014 mole) of DBU in 75 mL of DMF. This preparation differs from well-known literature preparations for pyrimidinedione rings in that sodium trimethylsilanolate and DBU were used rather than sodium hydride. The yield of title compound was 1.7 grams. The NMR spectrum was consistent with the proposed structure.

Step E 3-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

A solution of 7.5 grams (0.021 mole) of 3-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione, 3.4 grams (0.025 mole) of potassium carbonate, and 3.5 grams (0.025 mole) of methyl iodide in 200 mL of acetone was stirred at ambient temperature for about 18 hours. The reaction mixture was then concentrated under reduced pressure, and the residue was taken up in 200 mL of water. The mixture was extracted with two 100 mL portions of ethyl acetate. The combined extracts were washed with two 50 mL portions of an aqueous saturated sodium chloride solution. The organic layer was dried with magnesium sulfate, filtered, and concentrated under reduced pressure, yielding 6.9 grams of crude product. The dark oil was combined with 7.0 grams of crude product prepared by a similar route to yield a total of 13.9 grams of crude product. The crude product was purified by column chromatography on silica gel, yielding 10.0 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step F 3-(4-chloro-6-fluoro-3-iodo-2-methoxyphenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

A solution of 4.0 grams (0.011 mole) of 3-(3-amino-4-chloro-6-fluoro-2-methoxyphenyl)-1-methyl-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione in 25 mL (0.300 mole) of concentrated hydrochloric acid was stirred and cooled in an ice bath. During a 15 minute period, 1.9 grams (0.013 mole) of sodium nitrite was added dropwise at a rate to maintain the reaction temperature at 15 °C. Upon completion of addition, the mixture was stirred for 20 minutes and then poured into 15.0 grams (0.090 mole) of potassium iodide. The reaction mixture was stirred for 30 minutes and then filtered. The filter cake was thoroughly washed with distilled water and then taken up in 150 mL of ethyl acetate. The resulting solution was dried with sodium sulfate and filtered. The filtrate was concentrated under reduced pressure to yield a brown solid. The solid was subjected to column chromatography on silica gel. Elution was accomplished using 5:1 heptane and ethyl acetate. The product-containing fractions were combined and concentrated under reduced pressure, yielding 3.0 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step G 3-(4-chloro-6-fluoro-2-hydroxy-3-iodophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

Under a nitrogen atmosphere, a stirred solution of 3.0 grams (0.006 mole) of 3-(4-chloro-6-fluoro-3-iodo-2-methoxyphenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 75 mL of methylene chloride was cooled in a dry ice/acetone bath and 22.0 mL (0.022 mole) of 1M boron tribromide (in methylene chloride) was added dropwise during a 20 minute period. Upon completion of addition, the reaction mixture was allowed to warm to ambient temperature were it stirred for about one hour. At the conclusion of this period, the reaction mixture was poured into 200 mL of water and extracted with two 50 mL portions of methylene chloride. The combined extracts were washed with one 100 mL portion of an aqueous saturated sodium chloride solution, dried with sodium sulfate, and filtered. The filtrate was concentrated under reduced pressure, yielding 2.6 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step H Compound 280

Under a nitrogen atmosphere, a solution of 1.5 grams (0.003 mole) of 3-(4-chloro-6-fluoro-2-hydroxy-3-iodophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione, 0.41 gram (0.004 mole) of phenylacetylene, and 0.71 gram (0.007 mole) of triethylamine in 25 mL of DMF was stirred. To this was added 0.09 gram (0.00013 mole) of dichlorobis(triphenylphosphine)pallidium (II) and 0.05 gram (0.00026 mole) of copper (I) iodide. Upon completion of addition, the reaction mixture was heated to 70 °C where it stirred for 2.5 hours. After this time, the reaction mixture was cooled to ambient temperature and then poured into 150 mL of an aqueous 10% ammonium chloride solution. The resulting precipitate was collected by filtration and washed with water. The precipitate was taken up in 120 mL of ethyl acetate. The resulting solution was dried with sodium sulfate and filtered. The filtrate was concentrated under reduced pressure to a brown solid. The solid was recrystallized using 1:1 chloroform and petroleum ether, yielding 0.31 gram of Compound 280. The mother liquor was concentrated to a residue. The residue was recrystallized using petroleum ether to yield an additional 0.21 gram of Compound 280, m.p. 215-216 °C. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 5

SYNTHESIS OF 3-(4-CHLORO-6-FLUORO-2-TRIFLUOROMETHYLBENZIMIDAZOL-7-YL)-1-METHYL-6-TRIFLUOROMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE

(Compound 365)

A stirred solution of 3.0 grams (0.0085 mole) of 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 15.0 mL of trifluoroacetic acid was heated to 65 °C where it stirred for one hour. At the conclusion of this period, the reaction mixture was analyzed by TLC, which indicated that the reaction was not complete. The reaction mixture was stirred at 65 °C for an additional two hours. After this time, the reaction mixture was again analyzed by TLC, which indicated that the reaction was complete. The reaction mixture was allowed to cool to ambient temperature and then poured into 200 mL of water. The resulting mixture was allowed to stand at ambient temperature for about 18 hours. At the conclusion of this period, the resulting solid was collected by filtration and washed with water followed by heptane. The filter cake was dried under vacuum, yielding 3.6 grams of Compound 365, m.p. 130 °C. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 6

SYNTHESIS OF 3-(4-CHLORO-2-ETHYL-6-FLUOROBENZIMIDAZOL-7-YL)-1-METHYL-6-TRIFLUOROMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE

(COMPOUND 367)

Step A 3-(4-chloro-2,6-difluorophenyl)-1-methyl-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione

Under a nitrogen atmosphere, a solution of 32.0 grams (0.900 mole) of sodium hydride (60% by weight) in 250 mL of DMF was vigorously stirred and cooled in an ice bath. To this a solution of 133.0 grams (0.726 mole) of ethyl 3-amino-4,4,4-trifluorocrotonate in 150 mL of DMF was added dropwise at a rate to maintain the reaction mixture temperature at about 5 °C. Upon completion of addition, a solution of 156.3 grams (0.663 mole) of ethyl N-(4-chloro-2,6-difluorophenyl)carbamate in 250 mL of DMF was added dropwise. Upon completion of addition, the mixture was

removed from the ice bath and heated to 130 °C where it stirred for 3.5 hours. After this time, the mixture was analyzed by gas chromatography (GC), which indicated that only a slight amount of the starting material was left. The mixture was cooled to 5 °C and 83.0 mL (1.333 moles) of methyl iodide was added dropwise at a rate to maintain the reaction mixture temperature below 20 °C. Upon completion of addition, the reaction mixture was allowed to warm to ambient temperature where it stirred for about 18 hours. At the conclusion of this period, the reaction mixture was filtered through diatomaceous earth. The filtrate was concentrated under reduced pressure to yield a dark viscous oil. The oil was taken up in methylene chloride and washed with three 1000 mL portions of water followed by one 1000 mL portion of an aqueous saturated sodium chloride solution. The organic layer was dried with magnesium sulfate, filtered, and concentrated under reduced pressure, yielding 223.8 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step B 3-(4-chloro-2,6-difluoro-5-nitrophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

A stirred solution of 211.0 grams (0.619 mole) of 3-(4-chloro-2,6-difluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 600 mL of concentrated sulfuric acid was cooled to less than 10 °C, and 44 mL (0.689 mole) of aqueous 70% nitric acid was added dropwise at a rate to maintain the reaction temperature below 10 °C. Upon completion of addition, the reaction mixture was analyzed by GC, which indicated the reaction was incomplete. The reaction was allowed to warm to ambient temperature and an additional 5 mL (0.078 mole) of aqueous 70% nitric acid was added. The reaction mixture was again analyzed by GC, which indicated the reaction was complete. The reaction mixture was poured into ice-water. The resulting solid was collected by filtration, washed with water, and then taken up in 600 mL of methylene chloride. The resulting solution was washed with two 600 mL portions of water, one 600 mL portion of an aqueous saturated sodium bicarbonate solution, and one 600 mL portion of an aqueous saturated sodium chloride solution. The organic layer was separated, dried with magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure, yielding a waxy tan solid. The solid was triturated with heptane and allowed to stand for about 72 hours. At the conclusion of this period, the solid was collected by filtration,

washed with heptane, and dried under reduced pressure, yielding 201.4 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step C 3-(6-amino-4-chloro-2-fluoro-5-nitrophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

To stirred solution of 200 grams (0.519 mole) of 3-(4-chloro-2,6-difluoro-5-nitrophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 1000 mL of dioxane was added 150 mL (1.091 moles) of triethylamine in one portion. Upon completion of addition, the mixture was vigorously stirred and 400 grams (5.189 moles) of ammonium acetate was added in one portion. The reaction mixture was heated to 90 °C where it stirred for two hours. The reaction mixture was allowed to cool to ambient temperature where it stirred for about 18 hours. The resulting suspension was collected by filtration and washed with dioxane. The filtrate was concentrated under reduced pressure to yield a viscous dark oil. The oil was poured into ice-water. The resulting solid was collected by filtration and washed with water. The solid was dried under reduced pressure and then at ambient temperature for about 18 hours, yielding 195.1 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step D 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione and 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

A solution of 278.0 grams (1.232.moles) of tin(II) chloride dihydrate, 264.0 grams (4.936 moles) of ammonium chloride, 400 mL of water. and 800 mL of ethanol was vigorously stirred, and 157.4 grams (0.411 mole) of 3-(6-amino-4-chloro-2-fluoro-5-nitrophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione was added. Upon completion of addition, the reaction mixture was heated to 83-85 °C where it stirred for 18 hours. After this time the reaction mixture was allowed to cool to ambient temperature. The resultant solid by-product was collected by filtration and washed with ethanol. The combined filtrate and wash was concentrated under reduced pressure to yield a suspension of additional by-product. The suspension was taken up in ethyl acetate and the resultant emulsion was filtered through a pad of diatomaceous earth. The filter cake was washed with ethyl acetate, and the combined organics were washed with three 200 mL portions of water. The organic

layer was dried with magnesium sulfate, filtered, and concentrated under reduced pressure to a brown residue. The residue was triturated with heptane and allowed to stand for about five days. The resultant solid was collected by filtration and dried, yielding 144.4 grams of crude product. The crude product was combined with material prepared by a similar route, yielding a total of 157.8 grams of material. The combined product was subjected to column chromatography on silica gel, yielding 83.2 grams of an orange solid. The solid was slurried with warm ethyl acetate, and the insoluble product was collected by filtration. The product was washed with ethyl acetate, and the wash and filtrate from above were combined. The process of concentrating the filtrate, and slurrying the solid residue was repeated twice more, yielding a total of 51.9 grams of title compound. The NMR spectrum was consistent with the proposed structure.

An alternate method for preparing 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione is the following:

A solution of 19.2 grams (0.050 mole) of 3-(6-amino-4-chloro-2-fluoro-5-nitrophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione, 3.0 grams (0.056 mole) of ammonium chloride, and 50 mL of water in 100 mL of ethanol was stirred, and 11.2 grams (0.201 mole) of iron powder (325 mesh) was added in one portion. Upon completion of addition, the reaction mixture was heated at reflux for one hour. The reaction mixture was allowed to cool to ambient temperature, then it was filtered through diatomaceous earth to remove the iron powder. The filter cake was washed with 200 mL of acetone, and the wash was combined with the filtrate. The combination was stirred with decolorizing carbon and filtered. The filtrate was concentrated under reduced pressure, yielding a dark brown oil. The oil was then taken up in 200 mL of methylene chloride and washed with three 100 mL portions of an aqueous saturated sodium bicarbonate solution. The organic layer was dried with magnesium sulfate, filtered, and concentrated under reduced pressure, yielding 12.8 grams of title compound. The NMR spectrum was consistent with the proposed structure.

Step E Compound 367

A stirred solution of 1.0 grams (0.0028 mole) of 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione and 0.28 mL

(0.0035 mole) of pyridine in 10 mL chloroform was cooled to 5 °C and 0.27 mL (0.0031 mole) of propionyl chloride was added dropwise. Upon completion of addition, the mixture was allowed to warm to ambient temperature were it stirred for about 18 hours. The mixture was cooled to 5 °C and 5.0 mL (0.054 mole) of phosphorous oxychloride was added in one portion. Upon completion of addition, the reaction mixture was allowed to warm to ambient temperature where it stirred for about 18 hours. At the conclusion of this period, the reaction mixture was poured into 200 mL of cold water, the resulting mixture was stirred for one hour, then it was extracted with three 50 mL portions of chloroform. The combined extracts were dried with magnesium sulfate and filtered. The filtrate was concentrated under reduced pressure, yielding 0.15 gram of an orange residue. The aqueous layer was made basic with an aqueous saturated sodium bicarbonate solution to a pH of 3-4. The resulting mixture was extracted with three 50 mL portions of methylene chloride. The extracts were combined, dried with magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure, yielding 0.70 gram of a yellow residue. The yellow residue was triturated with hot heptane. The resulting solid was collected by filtration and washed with heptane, yielding 0.67 gram of Compound 367, m.p. 150-155 °C. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 7

SYNTHESIS OF 3-(2-T-BUTYL-4-CHLORO-6-FLUOROBENZIMIDAZOL-7-YL)-1-METHYL-6-TRIFLUOROMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE (Compound 369)

To a stirred solution of 1.0 grams (0.0028 mole) of 3-(5,6-diamino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione , 15.0 mL of ethanol, and 4 mL of 5M hydrochloric acid was added 1.2 mL (0.0057 mole) of 2,2,6,6-tetramethyl-3,5-heptanedione. Upon completion of addition, the reaction mixture was heated to reflux where it stirred for ten minutes. At the conclusion of this period, the reaction mixture was analyzed by TLC, which indicated that the reaction was not complete. The reaction mixture was stirred at reflux for an additional two hours. After this time, the reaction mixture was again analyzed by TLC, which again indicated that the reaction was still not complete. As a result, an additional 1.0 mL

(0.0048 mole) of 2,2,6,6-tetramethyl-3,5-heptanedione was added. Upon completion of addition, the reaction mixture was stirred at reflux for three days. At the conclusion of this period, more ethanol was added to replace that which evaporated, and the reaction mixture was analyzed by TLC for a third time. The reaction mixture was allowed to cool to ambient temperature, poured into 100 mL of an aqueous saturated sodium bicarbonate solution, and 100 mL of chloroform was added. The aqueous layer was separated and washed with two 100 mL portions of chloroform. The chloroform layer and washes were combined, dried with magnesium sulfate, and filtered. The filtrate was treated with decolorizing carbon and stirred. The mixture was filtered and concentrated under reduced pressure to yield a red oil. The oil was taken up in heptane. The resulting solid was collected by filtration and washed with heptane to yield a tan solid. The solid was purified by column chromatography on silica gel, yielding 0.36 gram of Compound 369, m.p. 125-130 °C. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 8

SYNTHESIS OF 3-(7-CHLORO-5-FLUORO-2-TRIFLUOROMETHYLINDOL-4-YL)-1-METHYL-6-TRIFLUOROMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE

(Compound 500)

Step A 3-[5-(1-trifluoromethylethylidenehydrazino)-4-chloro-2-fluorophenyl]-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione

A solution of 3.37 grams (0.010 mole) of 3-(5-amino-4-chloro-2-fluorophenyl)-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 80 mL of concentrated hydrochloric acid was stirred at 25 °C for 20 minutes. After this time, the solution was cooled to 10 °C and a solution of 0.69 gram (0.010 mole) of sodium nitrite in 10 mL of water was slowly added. Upon completion of addition, the mixture was stirred for one hour at 10 °C and then a solution of 5.64 grams (0.025 mole) of tin (II) chloride dihydrate in 40 mL of concentrated hydrochloric acid was slowly added. Upon completion of addition, the reaction mixture was warmed to 25 °C where it stirred for one hour. At the conclusion of this period, 1.12 grams (0.010 mole) of trifluoroacetone was added and the resulting solid was collected by filtration,

yielding 3.13 grams of title compound, m.p. 213-214 °C. The NMR spectrum was consistent with the proposed structure.

Step B Compound 500

A stirred solution of 2.0 grams (0.0044 mole) of 3-[5-(1-trifluoromethylethylidenehydrazino)-4-chloro-2-fluorophenyl]-1-methyl-6-trifluoromethyl-2,4(1H,3H)-pyrimidinedione in 80 mL of polyphosphoric acid was heated at 80 °C for 20 minutes. After this time, the reaction mixture was allowed to cool to 25 °C where it was diluted with water. The resulting solid was collected by filtration, yielding 0.73 gram of Compound 500, m.p. 208-210 °C. The NMR spectrum was consistent with the proposed structure.

EXAMPLE 9

SYNTHESIS OF 3-(7-CHLORO-2-ETHOXYCARBONYLINDOL-4-YL)-4,5,6,7-TETRAHYDRO-1H-ISOINDOLE-1,3(2H)-DIONE

(Compound 595)

Step A 3-(1-ethoxycarbonylethylidenehydrazino)-4-chloronitrobenzene

This compound was prepared in the manner of Step A, Example 1, using, 17.25 grams (0.10 mole) of 2-chloro-5-nitroaniline, 6.9 grams (0.10 mole) of sodium nitrite, 56.4 grams (0.25 mole) of tin (II) chloride dihydrate, 11.61 grams (0.10 mole) of ethyl pyruvate, 30 mL of water, and 100 mL of concentrated hydrochloric acid. This preparation differs in that ethyl pyruvate was used rather than trifluoroacetone. The yield of title compound was 19.4 grams. The NMR spectrum was consistent with the proposed structure.

Step B 7-chloro-2-ethoxycarbonyl-4-nitroindole

This compound was prepared in the manner of Step B, Example 8, using 14.0 grams (0.050 mole) of 3-(1-ethoxycarbonylethylidenehydrazino)-4-chloronitrobenzene in 100 mL of polyphosphoric acid. The yield of title compound was 0.4 gram. The NMR spectrum was consistent with the proposed structure.

Step C 7-amino-4-chloro-2-ethoxycarbonylindole

A stirred solution of 2.68 grams (0.01 mole) of 4-chloro-2-ethoxycarbonyl-7-nitroindole, 80 mL of acetic acid, and 15 mL of water was heated to 65 °C, and 18.3 grams (0.048 mole) of iron powder was slowly added during a 20

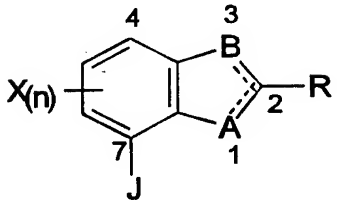
minute period. Upon completion of addition, the reaction mixture was allowed to cool to 25 °C where it stirred for one hour. After this time, the reaction mixture was poured into water, and the resulting mixture was filtered through diatomaceous earth. The filter cake was washed thoroughly with ethyl acetate. The organic layer was dried with magnesium sulfate and filtered. The filtrate was concentrated under reduced pressure a residue. The residue was purified by column chromatography, yielding 0.4 gram of title compound. The NMR spectrum was consistent with the proposed structure.

Step D Compound 595

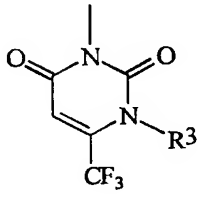
A stirred solution of 0.4 gram (0.0016 mole) of 7-amino-4-chloro-2-ethoxycarbonylindole and 0.26 gram (0.0016 mole) of 3,4,5,6-tetrahydrophhalic anhydride in 80 mL of acetic acid was heated at reflux for about 18 hours. After this time, the reaction mixture was extracted with several portions of diethyl ether. The organic extracts were combined, dried with magnesium sulfate, and filtered. The filtrate was concentrated under reduced pressure to a residue. The residue was purified by column chromatography on silica gel, yielding 0.47 gram of Compound 595. The NMR spectrum was consistent with the proposed structure.

Table 1

Benzoxazoles

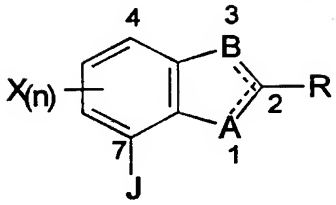


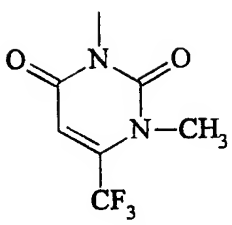
where A is nitrogen double bonded to position 2 and B is O; J is

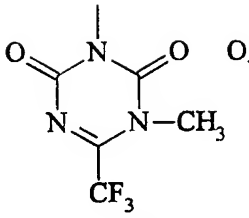


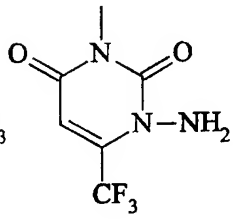
Compound No.	X	R	R3
1	4-Cl, 6-F	CH_3	CH_3
2	4-Cl, 6-F	CH_3	C_2H_5
3	4-Cl, 6-F	CH_3	CH_2CN
4	4-Cl, 6-F	CH_3	$CH_2CH=CH_2$
5	4-Cl, 6-F	CH_3	NH_2
6	4-Cl, 6-F	CH_3	$CH_2C\equiv CH$
7	4-Cl, 6-F	CH_3	C_3H_7
8	4-Cl, 6-F	CH_3	CH_2OCH_3
9	4-Cl, 6-F	CH_3	$CH_2CO_2C_2H_5$

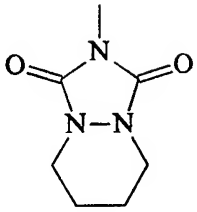
Table 2

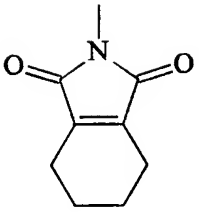


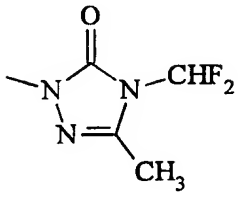

J1

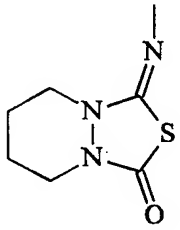

J2


J3


J4


J5


J6


J7

No.	A	B	Double Bond Posit'n	X	R	J
10	N	O	1-2	4-Cl	CH_3	J1
11	N	O	1-2	4-Cl	C_2H_5	J1
12	N	O	1-2	4-Cl	$CH(CH_3)_2$	J1
13	N	O	1-2	4,6-Cl_2	CH_3	J1
14	N	O	1-2	4,6-Cl_2	C_2H_5	J1
15	N	O	1-2	4,6-Cl_2	C_2H_5	J1
16	N	O	1-2	4-Br, 6-F	CH_3	J1
17	N	O	1-2	4-CF_3,6-F	CH_3	J1
18	N	O	1-2	4,6-F_2	CH_3	J1
19	N	O	1-2	4-CN, 6-F	CH_3	J1
20	N	O	1-2	4-OCF_3,6-F	CH_3	J1
21	N	O	1-2	4-Br, 6-F	C_2H_5	J1
22	N	O	1-2	4-CN, 6-F	C_2H_5	J1
23	N	O	1-2	4-CN, 6-F	$CH(CH_3)_2$	J1
24	N	O	1-2	4-CH_3, 6-F	CH_3	J1
25	N	O	1-2	4-Cl, 6-F	C_2H_5	J1
26	N	O	1-2	4-Cl, 6-F	C_3H_7	J1
27	N	O	1-2	4-Cl, 6-F	C_4H_9	J1
28	N	O	1-2	4-Cl, 6-F	$CH(CH_3)_2$	J1
29	N	O	1-2	4-Cl, 6-F	$CH_2CH(CH_3)_2$	J1

	30	N	O	1-2	4-Cl, 6-F	$C(CH_3)_3$	J1
	31	N	O	1-2	4-Cl, 6-F	phenyl	J1
	32	N	O	1-2	4-Cl, 6-F	phenylmethyl	J1
	33	N	O	1-2	4-Cl, 6-F	CF_3	J1
5	34	N	O	1-2	4-Cl, 6-F	CCl_2	J1
	35	N	O	1-2	4-Cl, 6-F	Cl	J1
	36	N	O	1-2	4-Cl, 6-F	OH	J1
	37	N	O	1-2	4-Cl, 6-F	Br	J1
	38	N	O	1-2	4-Cl, 6-F	NH_2	J1
10	39	N	O	1-2	4-Cl, 6-F	$NHCH_3$	J1
	40	N	O	1-2	4-Cl, 6-F	$N(CH_3)_2$	J1
	41	N	O	1-2	4-Cl, 6-F	$NHCH_2CO_2CH_3$	J1
	42	N	O	1-2	4-Cl, 6-F	$NHSO_2CH_3$	J1
	43	N	O	1-2	4-Br, 6-F	$NHCOCH_3$	J1
15	44	N	O	1-2	4-Cl, 6-F	morpholino	J1
	45	N	O	1-2	4-Cl, 6-F	$NHSO_2C_6H_5$	J1
	46	N	O	1-2	4-Cl, 6-F	$NHSO_2CH_2C_6H_5$	J1
	47	N	O	1-2	4-Cl, 6-F	$N(CH_3)SO_2CH_3$	J1
	48	N	O	1-2	4-Cl, 6-F	$NHPO(OCH_3)_2$	J1
20	49	N	O	1-2	4-Br, 6-F	$CH_2CO_2CH_3$	J1
	50	N	O	1-2	4-Cl, 6-F	$C_2H_4CO_2CH_3$	J1
	51	N	O	1-2	4-Cl, 6-F	$CH=CHCO_2CH_3$	J1
	52	N	O	1-2	4-Cl, 6-F	$CH=C(Cl)CO_2CH_3$	J1
	53	N	O	1-2	4-Cl, 6-F	$CH_2CH(Cl)CO_2CH_3$	J1
25	54	N	O	1-2	4-Cl, 6-F	OCH_3	J1
	55	N	O	1-2	4-Cl, 6-F	OC_2H_5	J1
	56	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)_2$	J1
	57	N	O	1-2	4-Cl, 6-F	$OCH_2CH=CH_2$	J1
	58	N	O	1-2	4-Cl, 6-F	$OCH_2C(CH_3)=CH_2$	J1
30	59	N	O	1-2	4-Cl, 6-F	OCH_2CCH	J1
	60	N	O	1-2	4-Cl, 6-F	$OCH_2CO_2C_2H_5$	J1
	61	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CO_2CH_3$	J1
	62	N	O	1-2	4-Cl, 6-F	OCH_2CN	J1
	63	N	O	1-2	4-Cl, 6-F	OCH_2CONH_2	J1
35	64	N	O	1-2	4-Cl, 6-F	$OCH_2CONHCH_3$	J1
	65	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CONH_2$	J1
	66	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CONHCH_3$	J1
	67	N	O	1-2	4-Cl, 6-F	OCH_2CO_2H	J1
	68	N	O	1-2	4-Cl, 6-F	phenoxy	J1
40	69	N	O	1-2	4-Cl, 6-F	$p\text{-}OC_6H_4OCH(CH_3)CO_2CH_3$	J1
	70	N	O	1-2	4-Cl, 6-F	4-chlorophenoxy	J1
	71	N	O	1-2	4-Cl, 6-F	phenylmethoxy	J1
	72	N	O	1-2	4-Cl, 6-F	CN	J1
	73	N	O	1-2	4-Cl, 6-F	CO_2CH_3	J1
45	74	N	O	1-2	4-Cl, 6-F	CO_2H	J1
	75	N	O	1-2	4-Cl, 6-F	CO_2Na	J1
	76	N	O	1-2	4-Cl, 6-F	$CONH_2$	J1
	77	N	O	1-2	4-Cl, 6-F	$CONHCH_3$	J1
	78	N	O	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J1
50	79	N	O	1-2	4-Cl, 6-F	$CONHSO_2CH_3$	J1

	80	N	O	1-2	4-Cl, 6-F	CO_2NHOCH_3	J1
	81	N	O	1-2	4-Cl, 6-F	SCH_3	J1
	82	N	O	1-2	4-Cl, 6-F	$SCH_2CO_2CH_3$	J1
	83	N	O	1-2	4-Cl, 6-F	SCH_2CONH_2	J1
5	84	N	O	1-2	4-Cl, 6-F	SO_2CH_3	J1
	85	N	O	1-2	4-Cl, 6-F	SH	J1
	86	N	O	1-2	4-Cl, 6-F	CH_2OH	J1
	87	N	O	1-2	4-Cl, 6-F	$CH(CH_3)OH$	J1
	88	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J1
10	89	N	O	1-2	4-Cl, 6-F	C_2H_4OH	J1
	90	N	O	1-2	4-Cl, 6-F	$CH_2CH(CH_3)OH$	J1
	91	N	O	1-2	4-Cl, 6-F	$CH_2C(CH_3)_2OH$	J1
	92	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J1
	93	N	O	1-2	4-Cl, 6-F	$CH(CH_3)_2OCOCH_3$	J1
15	94	N	O	1-2	4-Cl, 6-F	$CH(CH_3)OCOCH_3$	J1
	95	N	O	1-2	4-Cl, 6-F	$CHBr_2$	J1
	96	N	O	1-2	4-Br, 6-F	CH_2OCH_3	J1
	97	N	O	1-2	4-Cl, 6-F	CH_2OCH_2CCH	J1
	98	N	O	1-2	4-Br, 6-F	NH_2	J1
20	99	N	O	1-2	4-Br, 6-F	phenoxymethyl	J1
	100	N	O	1-2	4-Br, 6-F	$N(COCH_3)_2$	J1
	101	N	O	1-2	4-Br, 6-F	CH_2OCOCH_3	J1
	102	N	O	1-2	4-Br, 6-F	4-chlorophenoxymethyl	J1
	103	N	O	1-2	4-Br, 6-F	$CH(Ph)OCOCH_3$	J1
25	104	N	O	1-2	4-Br, 6-F	$C(CH_3)_2OCOCH_3$	J1
	105	N	O	1-2	4-Br, 6-F	CO_2H	J1
	106	N	O	1-2	4-Br, 6-F	OCH_2CCH	J1
	107	N	O	1-2	4-Br, 6-F	$OCH(CH_3)_2$	J1
	108	N	O	1-2	4-Br, 6-F	$NHSO_2CH_3$	J1
30	109	N	O	1-2	4-Br, 6-F	OCH_3	J1
	110	N	O	1-2	4-Br, 6-F	$OCH_2CH=CH_2$	J1
	111	N	O	1-2	4-Cl, 6-F	$(CH_3)(CN)OH$	J1
	112	N	O	1-2	4-Cl, 6-F	CH_3	J2
	113	N	O	1-2	4-Cl, 6-F	n-C_3H_7	J2
35	114	N	O	1-2	4-Cl, 6-F	i-C_3H_7	J2
	115	N	O	1-2	4-Cl, 6-F	t-C_4H_9	J2
	116	N	O	1-2	4-Cl, 6-F	C_2H_5	J2
	117	N	O	1-2	4-Cl, 6-F	$CH_2CO_2CH_3$	J2
	118	N	O	1-2	4-Cl, 6-F	phenoxymethyl	J2
40	119	N	O	1-2	4-Cl, 6-F	$CONHCH_3$	J2
	120	N	O	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J2
	121	N	O	1-2	4-Cl, 6-F	CO_2CH_3	J2
	122	N	O	1-2	4-Cl, 6-F	Phenyl	J2
	123	N	O	1-2	4-Cl, 6-F	SCH_3	J2
45	124	N	O	1-2	4-Cl, 6-F	CH_2OCH_3	J2
	125	N	O	1-2	4-Cl, 6-F	Benzyl	J2
	126	N	O	1-2	4-Cl, 6-F	4-chlorophenylmethyl	J2
	127	N	O	1-2	4-Cl, 6-F	SO_2CH_3	J2
	128	N	O	1-2	4-Cl, 6-F	CF_3	J2
50	129	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OCO_2CH_3$	J2

	130	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J2
	131	N	O	1-2	4-Cl, 6-F	CH_3	J3
	132	N	O	1-2	4-Cl, 6-F	$n\text{-}C_3H_7$	J3
	133	N	O	1-2	4-Cl, 6-F	$i\text{-}C_3H_7$	J3
5	134	N	O	1-2	4-Cl, 6-F	$t\text{-}C_4H_9$	J3
	135	N	O	1-2	4-Cl, 6-F	CH_2OH	J3
	136	N	O	1-2	4-Cl, 6-F	CH_2CH_2OH	J3
	137	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J3
	138	N	O	1-2	4-Cl, 6-F	$CONHCH_3$	J3
10	139	N	O	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J3
	140	N	O	1-2	4-Cl, 6-F	CO_2CH_3	J3
	141	N	O	1-2	4-Cl, 6-F	Phenyl	J3
	142	N	O	1-2	4-Cl, 6-F	SCH_3	J3
	143	N	O	1-2	4-Cl, 6-F	CH_2OCH_3	J3
15	144	N	O	1-2	4-Cl, 6-F	Benzyl	J3
	145	N	O	1-2	4-Cl, 6-F	4-chlorophenylmethyl	J3
	146	N	O	1-2	4-Cl, 6-F	SO_2CH_3	J3
	147	N	O	1-2	4-Cl, 6-F	CF_3	J3
	148	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OCO_2CH_3$	J3
20	149	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J3
	150	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OCH_3$	J3
	151	N	O	1-2	4-Cl, 6-F	C_2H_5	J3
	152	N	O	1-2	4-Cl, 6-F	CO_2Na	J3
	153	N	O	1-2	4-Cl, 6-F	$CONHSO_2CH_3$	J3
25	154	N	O	1-2	4-Cl, 6-F	$OCH_2CO_2CH_3$	J3
	155	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CO_2CH_3$	J3
	156	N	O	1-2	4-Cl, 6-F	$OCH_2CH{=}CH_2$	J3
	157	N	O	1-2	4-Cl, 6-F	OCH_2CCH	J3
	158	N	O	1-2	4-Cl, 6-F	OH	J3
30	159	N	O	1-2	4-Cl, 6-F	OCH_3	J3
	160	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)_2$	J3
	161	N	O	1-2	4-Cl, 6-F	CH_3	J4
	162	N	O	1-2	4-Cl, 6-F	$n\text{-}C_3H_7$	J4
	163	N	O	1-2	4-Cl, 6-F	$i\text{-}C_3H_7$	J4
35	164	N	O	1-2	4-Cl, 6-F	$t\text{-}C_4H_9$	J4
	165	N	O	1-2	4-Cl, 6-F	CH_2OH	J4
	166	N	O	1-2	4-Cl, 6-F	CH_2CH_2OH	J4
	167	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J4
	168	N	O	1-2	4-Cl, 6-F	$CONHCH_3$	J4
40	169	N	O	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J4
	170	N	O	1-2	4-Cl, 6-F	CO_2CH_3	J4
	171	N	O	1-2	4-Cl, 6-F	Phenyl	J4
	172	N	O	1-2	4-Cl, 6-F	SCH_3	J4
	173	N	O	1-2	4-Cl, 6-F	CH_2OCH_3	J4
45	174	N	O	1-2	4-Cl, 6-F	Benzyl	J4
	175	N	O	1-2	4-Cl, 6-F	4-chlorophenylmethyl	J4
	176	N	O	1-2	4-Cl, 6-F	SO_2CH_3	J4
	177	N	O	1-2	4-Cl, 6-F	CF_3	J4
	178	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OCO_2CH_3$	J4
50	179	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J4

180	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OCH_3$	J4
181	N	O	1-2	4-Cl, 6-F	C_2H_5	J4
182	N	O	1-2	4-Cl, 6-F	CO_2Na	J4
183	N	O	1-2	4-Cl, 6-F	$CONHSO_2CH_3$	J4
184	N	O	1-2	4-Cl, 6-F	$OCH_2CO_2CH_3$	J4
185	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CO_2CH_3$	J4
186	N	O	1-2	4-Cl, 6-F	$OCH_2CH=CH_2$	J4
187	N	O	1-2	4-Cl, 6-F	$OCH_2C\equiv CH$	J4
188	N	O	1-2	4-Cl, 6-F	OH	J4
189	N	O	1-2	4-Cl, 6-F	OCH_3	J4
190	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)_2$	J4
191	N	O	1-2	4-Cl, 6-F	CH_3	J5
192	N	O	1-2	4-Cl, 6-F	$n\text{-}C_3H_7$	J5
193	N	O	1-2	4-Cl, 6-F	$i\text{-}C_3H_7$	J5
194	N	O	1-2	4-Cl, 6-F	$t\text{-}C_4H_9$	J5
195	N	O	1-2	4-Cl, 6-F	CH_2OH	J5
196	N	O	1-2	4-Cl, 6-F	CH_2CH_2OH	J5
197	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J5
198	N	O	1-2	4-Cl, 6-F	$CONHCH_3$	J5
199	N	O	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J5
200	N	O	1-2	4-Cl, 6-F	CO_2CH_3	J5
201	N	O	1-2	4-Cl, 6-F	Phenyl	J5
202	N	O	1-2	4-Cl, 6-F	SCH_3	J5
203	N	O	1-2	4-Cl, 6-F	CH_2OCH_3	J5
204	N	O	1-2	4-Cl, 6-F	Benzyl	J5
205	N	O	1-2	4-Cl, 6-F	4-chlorophenylmethyl	J5
206	N	O	1-2	4-Cl, 6-F	SO_2CH_3	J5
207	N	O	1-2	4-Cl, 6-F	CF_3	J5
208	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2OCO_2CH_3$	J5
209	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J5
210	N	O	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OCH_3$	J5
211	N	O	1-2	4-Cl, 6-F	C_2H_5	J5
212	N	O	1-2	4-Cl, 6-F	CO_2Na	J5
213	N	O	1-2	4-Cl, 6-F	$CONHSO_2CH_3$	J5
214	N	O	1-2	4-Cl, 6-F	$OCH_2CO_2CH_3$	J5
215	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)CO_2CH_3$	J5
216	N	O	1-2	4-Cl, 6-F	$OCH_2CH=CH_2$	J5
217	N	O	1-2	4-Cl, 6-F	OCH_2CCH	J5
218	N	O	1-2	4-Cl, 6-F	OH	J5
219	N	O	1-2	4-Cl, 6-F	OCH_3	J5
220	N	O	1-2	4-Cl, 6-F	$OCH(CH_3)_2$	J5
221	O	CH	2-3	4-Cl	CH_3	J1
222	O	CH	2-3	4-Cl, 6-F	CH_3	J1
223	O	CH	2-3	4-Cl, 6-F	n-propyl	J1
224	O	CH	2-3	4-Cl, 6-F	isopropyl	J1
225	O	CH	2-3	4-Cl	n-butyl	J1
226	O	CH	2-3	4-Cl	t-butyl	J1
227	O	CH	2-3	4-Cl, 6-F	t-butyl	J1
228	O	CH	2-3	$4,6\text{-}F_2$	t-butyl	J1
229	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)C_3H_7$	J1

	230	O	CH	2-3	4-Cl, 6-F	$CH=CH_2$	J1
	231	O	CH	2-3	4-Cl, 6-F	$C(CH_3)=CH_2$	J1
	232	O	CH	2-3	4-Cl	CH_2Br	J1
	233	O	CH	2-3	4-Cl	$CHBr_2$	J1
5	234	O	CH	2-3	4-Cl, 6-F	$CH(Cl)CH_3$	J1
	235	O	CH	2-3	4-Cl, 6-F	$CH(F)CH_3$	J1
	236	O	CH	2-3	4-Cl, 6-F	CH_2CH_2Cl	J1
	237	O	CH	2-3	4-Cl, 6-F	CH_2CH_2F	J1
	238	O	CH	2-3	4-Cl	CH_2OH	J1
10	239	O	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J1
	240	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OH$	J1
	241	O	CH	2-3	4-Cl	$C(CH_3)_2OH$	J1
	242	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J1
	243	O	CH	2-3	4-Cl, 6-F	$CH_2CH(CH_3)OH$	J1
15	244	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OC(CH_3)_3$	J1
	245	O	CH	2-3	4-Cl, 6-F	$CH(OC_2H_5)_2$	J1
	246	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOCH_3$	J1
	247	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOCH(CH_3)_2$	J1
	248	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOPh$	J1
20	249	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCONHCH_3$	J1
	250	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCONHCH_2Ph$	J1
	251	O	CH	2-3	4-Cl	$C(CH_3)_2OCH_3$	J1
	252	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCH_2OCH_3$	J1
	253	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J1
25	254	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NH_2$	J1
	255	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J1
	256	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CH_2CN$	J1
	257	O	CH	2-3	4-Cl	$CH_2N(C_2H_5)_2$	J1
	258	O	CH	2-3	4-Cl	CH=NOH	J1
30	259	O	CH	2-3	4-Cl	$CH=NOCH_3$	J1
	260	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2OCOCH_3$	J1
	261	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2OCONHCH_3$	J1
	262	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2H$	J1
	263	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2CH_3$	J1
35	264	O	CH	2-3	4-Cl	Phenyl	J1
	265	O	CH	2-3	4-Cl	CHO	J1
	266	O	CH	2-3	4-Cl	CO_2H	J1
	267	O	CH	2-3	H	$CO_2C_2H_5$	J1
	268	O	CH	2-3	4-Cl	$CO_2C_2H_5$	J1
40	269	O	CH	2-3	4-Cl	$CONH_2$	J1
	270	O	CH	2-3	4-Cl	$CONHCH_3$	J1
	271	O	CH	2-3	4-Cl	$CON(CH_3)_2$	J1
	272	O	CH	2-3	4-Cl	$NHCO_2C(CH_3)_3$	J1
	273	O	CH	2-3	4-Cl, 6-F	$CONH_2$	J1
45	274	O	CH	2-3	4-Cl, 6-F	$CONH(CH_3)$	J1
	275	O	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J1
	276	O	CH	2-3	4-Cl, 6-F	CO_2H	J1
	277	O	CH	2-3	4-Cl, 6-F	CO_2CH_3	J1
	278	O	CH	2-3	4-Cl, 6-F	CH_2OH	J1
50	279	O	CH	2-3	4-Cl, 6-F	3,4-dimethoxyphenyl	J1

	280	O	CH	2-3	4-Cl, 6-F	Phenyl	J1
	281	O	CH	2-3	4-Cl, 6-F	CH_3	J2
	282	O	CH	2-3	4-Cl, 6-F	n-propyl	J2
	283	O	CH	2-3	4-Cl, 6-F	isopropyl	J2
5	284	O	CH	2-3	4-Cl, 6-F	t-butyl	J2
	285	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)C_3H_7$	J2
	286	O	CH	2-3	4-Cl, 6-F	$CH=CH_2$	J2
	287	O	CH	2-3	4-Cl, 6-F	$C(CH_3)=CH_2$	J2
	288	O	CH	2-3	4-Cl, 6-F	$CH(Cl)CH_3$	J2
10	289	O	CH	2-3	4-Cl, 6-F	$CH(F)CH_3$	J2
	290	O	CH	2-3	4-Cl, 6-F	CH_2CH_2Cl	J2
	291	O	CH	2-3	4-Cl, 6-F	CH_2CH_2F	J2
	292	O	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J2
	293	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OH$	J2
15	294	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J2
	295	O	CH	2-3	4-Cl, 6-F	$CH_2CH(CH_3)OH$	J2
	296	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OC(CH_3)_3$	J2
	297	O	CH	2-3	4-Cl, 6-F	$CH(OC_2H_5)_2$	J2
	298	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOCH_3$	J2
20	299	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOCH(CH_3)_2$	J2
	300	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCOPh$	J2
	301	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCONHCH_3$	J2
	302	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OCONHCH_2Ph$	J2
	303	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCH_2OCH_3$	J2
25	304	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J2
	305	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NH_2$	J2
	306	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J2
	307	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CH_2CN$	J2
	308	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2OCOCH_3$	J2
30	309	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2OCONHCH_3$	J2
	310	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2H$	J2
	311	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2CH_3$	J2
	312	O	CH	2-3	4-Cl, 6-F	$CONH_2$	J2
	313	O	CH	2-3	4-Cl, 6-F	$CONH(CH_3)$	J2
35	314	O	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J2
	315	O	CH	2-3	4-Cl, 6-F	CO_2H	J2
	316	O	CH	2-3	4-Cl, 6-F	CO_2CH_3	J2
	317	O	CH	2-3	4-Cl, 6-F	CH_2OH	J2
	318	O	CH	2-3	4-Cl, 6-F	3,4-dimethoxyphenyl	J2
40	319	O	CH	2-3	4-Cl, 6-F	Phenyl	J2
	320	O	CH	2-3	4-Cl, 6-F	CH_3	J3
	321	O	CH	2-3	4-Cl, 6-F	C_2H_5	J3
	322	O	CH	2-3	4-Cl, 6-F	$CH(Cl)CH_3$	J3
	323	O	CH	2-3	4-Cl, 6-F	$CH(F)CH_3$	J3
45	324	O	CH	2-3	4-Cl, 6-F	CH_2CH_2Cl	J3
	325	O	CH	2-3	4-Cl, 6-F	CH_2CH_2F	J3
	326	O	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J3
	327	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OH$	J3
	328	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J3
50	329	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCH_2OCH_3$	J3

330	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J3
331	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CH_2CN$	J3
332	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2CH_3$	J3
333	O	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J3
334	O	CH	2-3	4-Cl, 6-F	CH_3	J4
335	O	CH	2-3	4-Cl, 6-F	C_2H_5	J4
336	O	CH	2-3	4-Cl, 6-F	$CH(Cl)CH_3$	J4
337	O	CH	2-3	4-Cl, 6-F	$CH(F)CH_3$	J4
338	O	CH	2-3	4-Cl, 6-F	CH_2CH_2Cl	J4
339	O	CH	2-3	4-Cl, 6-F	CH_2CH_2F	J4
340	O	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J4
341	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OH$	J4
342	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J4
343	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCH_2OCH_3$	J4
344	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J4
345	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CH_2CN$	J4
346	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2CH_3$	J4
347	O	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J4
348	O	CH	2-3	4-Cl, 6-F	CH_3	J5
349	O	CH	2-3	4-Cl, 6-F	C_2H_5	J5
350	O	CH	2-3	4-Cl, 6-F	$CH(Cl)CH_3$	J5
351	O	CH	2-3	4-Cl, 6-F	$CH(F)CH_3$	J5
352	O	CH	2-3	4-Cl, 6-F	CH_2CH_2Cl	J5
353	O	CH	2-3	4-Cl, 6-F	CH_2CH_2F	J5
354	O	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J5
355	O	CH	2-3	4-Cl, 6-F	$CH(CH_3)OH$	J5
356	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J5
357	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCH_2OCH_3$	J5
358	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J5
359	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CH_2CN$	J5
360	O	CH	2-3	4-Cl, 6-F	$CH_2CH_2CO_2CH_3$	J5
361	O	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J5
362	NH	N	2-3	4-Cl, 6-F	H	J1
363	NH	N	2-3	4-Cl, 6-F	CH_3	J1
364	NH	N	2-3	4-Cl, 6-F	CHF_2	J1
365	NH	N	2-3	4-Cl, 6-F	CF_3	J1
366	NH	N	2-3	4-Cl, 6-F	$CClF_2$	J1
367	NH	N	2-3	4-Cl, 6-F	C_2H_5	J1
368	NH	N	2-3	4-Cl, 6-F	$i\text{-}C_3H_7$	J1
369	NH	N	2-3	4-Cl, 6-F	$t\text{-}C_4H_9$	J1
370	NH	N	2-3	4-Cl, 6-F	CH_2OCH_3	J1
371	NH	N	2-3	4-Cl, 6-F	$C(CH_3)_2OC(O)CH_3$	J1
372	NH	N	2-3	4-Cl, 6-F	$C_2H_4CO_2C_2H_5$	J1
373	NH	N	2-3	4-Cl, 6-F	Cyclohexyl	J1
374	NH	N	2-3	4-Cl, 6-F	Adamantyl	J1
375	NH	N	2-3	4-Cl, 6-F	Phenyl	J1
376	NH	N	2-3	4-Cl, 6-F	Benzyl	J1
377	NH	N	2-3	4-Cl, 6-F	$CH(CH_3)C_6H_5$	J1
378	NH	N	2-3	4-Cl, 6-F	$CH_2OC_6H_5$	J1
379	NH	N	2-3	4-Cl, 6-F	$C_2H_4C_6H_5$	J1

380	NH	N	2-3	4-Cl, 6-F	$C_3H_6C_6H_5$	J1
381	NH	N	2-3	4-Cl, 6-F	2-chlorophenylmethyl	J1
382	NH	N	2-3	4-Cl, 6-F	3-chlorophenylmethyl	J1
383	NH	N	2-3	4-Cl, 6-F	4-chlorophenylmethyl	J1
384	NH	N	2-3	4-Cl, 6-F	CF_2CF_3	J1
385	NH	N	2-3	4-Cl, 6-F	Furan-2-yl	J1
386	NH	N	2-3	4-Cl, 6-F	CH_2Cl	J1
387	NH	N	2-3	4-Cl, 6-F	$C(CH_3)_2CH_2Cl$	J1
388	NH	N	2-3	4-Cl, 6-F	OC_2H_5	J1
389	N	NH	1-2	4-Cl, 6-F	CH_3	J1
390	N	NH	1-2	4-Cl, 6-F	C_2H_5	J1
391	N	NH	1-2	4-Cl, 6-F	isopropyl	J1
392	N	NH	1-2	4-Cl, 6-F	t-butyl	J1
393	N	NH	1-2	4-Cl, 6-F	CF_3	J1
394	N	NH	1-2	4-Cl, 6-F	CF_2CF_3	J1
395	N	NCH_3	1-2	4-Cl, 6-F	CH_3	J1
396	N	NCH_3	1-2	4-Cl, 6-F	C_2H_5	J1
397	N	NCH_3	1-2	4-Cl, 6-F	isopropyl	J1
398	N	NCH_3	1-2	4-Cl, 6-F	t-butyl	J1
399	N	NCH_3	1-2	4-Cl, 6-F	CF_3	J1
400	N	NCH_3	1-2	4-Cl, 6-F	CF_2CF_3	J1
401	N	NCH_3	1-2	4-Cl, 6-F	$CO_2CH_2CH_3$	J1
402	N	NC_2H_5	1-2	4-Cl, 6-F	CH_3	J1
403	N	NC_2H_5	1-2	4-Cl, 6-F	C_2H_5	J1
404	NH	NH	—	4-NO_2, 6-F	CF_3	J1
405	$N^- H_3N^+CH(CH_3)_2$	N	2-3	4-Cl, 6-F	CH_3	J1
406	NCH_3	N	2-3	4-Cl, 6-F	CF_3	J1
407	NCH_3	NC_2H_5	1-2	4-Cl, 6-F	isopropyl	J1
408	N	NC_2H_5	1-2	4-Cl, 6-F	t-butyl	J1
409	N	NC_2H_5	1-2	4-Cl, 6-F	CF_3	J1
410	N	NC_2H_5	1-2	4-Cl, 6-F	CF_2CF_3	J1
411	N	NC_4H_9	1-2	4-Cl, 6-F	CH_3	J1
412	N	NC_4H_9	1-2	4-Cl, 6-F	C_2H_5	J1
413	N	NC_4H_9	1-2	4-Cl, 6-F	isopropyl	J1
414	N	NC_4H_9	1-2	4-Cl, 6-F	t-butyl	J1
415	N	NC_4H_9	1-2	4-Cl, 6-F	CF_3	J1
416	N	NC_4H_9	1-2	4-Cl, 6-F	CF_2CF_3	J1
417	N	NCH_2OCH_3	1-2	4-Cl, 6-F	CH_3	J1
418	N	NCH_2OCH_3	1-2	4-Cl, 6-F	C_2H_5	J1
419	N	NCH_20CH_3	1-2	4-Cl, 6-F	isopropyl	J1
420	N	NCH_20CH_3	1-2	4-Cl, 6-F	t-butyl	J1
421	N	NCH_2OCH_3	1-2	4-Cl, 6-F	CF_3	J1
422	N	NCH_2OCH_3	1-2	4-Cl, 6-F	CF_2CF_3	J1
423	N	NCO_2CH_3	1-2	4-Cl, 6-F	CH_3	J1
424	N	NCO_2CH_3	1-2	4-Cl, 6-F	C_2H_5	J1
425	N	NCO_2CH_3	1-2	4-Cl, 6-F	isopropyl	J1
426	N	NCO_2CH_3	1-2	4-Cl, 6-F	t-butyl	J1
427	N	NCO_2CH_3	1-2	4-Cl, 6-F	CF_3	J1
428	N	NCO_2CH_3	1-2	4-Cl, 6-F	CF_2CF_3	J1

	429	N	NSO_2CH_3	1-2	4-Cl, 6-F	CH_3	J1
	430	N	NSO_2CH_3	1-2	4-Cl, 6-F	C_2H_5	J1
	431	N	NSO_2CH_3	1-2	4-Cl, 6-F	isopropyl	J1
	432	N	NSO_2CH_3	1-2	4-Cl, 6-F	t-butyl	J1
5	433	N	NSO_2CH_3	1-2	4-Cl, 6-F	CF_3	J1
	434	N	NSO_2CH_3	1-2	4-Cl, 6-F	CF_2CF_3	J1
	435	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	CH_3	J1
	436	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	C_2H_5	J1
	437	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	isopropyl	J1
10	438	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	t-butyl	J1
	439	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	CF_3	J1
	440	N	NCH_2CHCH_2	1-2	4-Cl, 6-F	CF_2CF_3	J1
	441	N	NCH_2CCH	1-2	4-Cl, 6-F	CH_3	J1
	442	N	NCH_2CCH	1-2	4-Cl, 6-F	C_2H_5	J1
15	443	N	NCH_2CCH	1-2	4-Cl, 6-F	isopropyl	J1
	444	N	NCH_2CCH	1-2	4-Cl, 6-F	t-butyl	J1
	445	N	NCH_2CCH	1-2	4-Cl, 6-F	CF_3	J1
	446	N	NCH_2CCH	1-2	4-Cl, 6-F	CF_2CF_3	J1
	447	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	CH_3	J1
20	448	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	C_2H_5	J1
	449	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	isopropyl	J1
	450	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	t-butyl	J1
	451	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	CF_3	J1
	452	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	CF_2CF_3	J1
25	453	N	NCF_3	1-2	4-Cl, 6-F	CH_3	J1
	454	N	NCF_3	1-2	4-Cl, 6-F	C_2H_5	J1
	455	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	isopropyl	J1
	456	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	t-butyl	J1
	457	N	NCH_2CO_2Me	1-2	4-Cl, 6-F	CF_3	J1
30	458	N	NCF_3	1-2	4-Cl, 6-F	CF_2CF_3	J1
	459	NH	N	2-3	4-Cl, 6-F	CH_3	J2
	460	NH	N	2-3	4-Cl, 6-F	C_2H_5	J2
	461	NH	N	2-3	4-Cl, 6-F	isopropyl	J2
	462	NH	N	2-3	4-Cl, 6-F	t-butyl	J2
35	463	NH	N	2-3	4-Cl, 6-F	CF_3	J2
	464	NH	N	2-3	4-Cl, 6-F	CF_2CF_3	J2
	465	NH	N	2-3	4-Cl, 6-F	CH_3	J3
	466	NH	N	2-3	4-Cl, 6-F	C_2H_5	J3
	467	NH	N	2-3	4-Cl, 6-F	isopropyl	J3
40	468	NH	N	2-3	4-Cl, 6-F	t-butyl	J3
	469	NH	N	2-3	4-Cl, 6-F	CF_3	J3
	470	NH	N	2-3	4-Cl, 6-F	CF_2CF_3	J3
	471	NH	N	2-3	4-Cl, 6-F	CH_3	J4
	472	NH	N	2-3	4-Cl, 6-F	C_2H_5	J4
45	473	NH	N	2-3	4-Cl, 6-F	isopropyl	J4
	474	NH	N	2-3	4-Cl, 6-F	t-butyl	J4
	475	NH	N	2-3	4-Cl, 6-F	CF_3	J4
	476	NH	N	2-3	4-Cl, 6-F	CF_2CF_3	J4
	477	NH	N	2-3	4-Cl, 6-F	CH_3	J5
50	478	NH	N	2-3	4-Cl, 6-F	C_2H_5	J5

479	NH	N	2-3	4-Cl, 6-F	isopropyl	J5
480	NH	N	2-3	4-Cl, 6-F	t-butyl	J5
481	NH	N	2-3	4-Cl, 6-F	CF_3	J5
482	NH	N	2-3	4-Cl, 6-F	CF_2CF_3	J5
483	NH	NH	1-2	4-Cl, 6-F	CH_3	J1
484	CH	NH	1-2	4-Cl, 6-F	$n\text{-}C_3H_7$	J1
485	CH	NH	1-2	4-Cl, 6-F	$i\text{-}C_3H_7$	J1
486	CH	NH	1-2	4-Cl, 6-F	$t\text{-}C_4H_9$	J1
487	CH	NH	1-2	4-Cl, 6-F	CH_2OH	J1
488	CH	NH	1-2	4-Cl, 6-F	CH_2CH_2OH	J1
489	CH	NH	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J1
490	CH	NH	1-2	4-Cl, 6-F	$CONHCH_3$	J1
491	CH	NH	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J1
492	CH	NH	1-2	4-Cl, 6-F	CO_2CH_3	J1
493	CH	NH	1-2	4-Cl, 6-F	$CO_2CH_2CH_3$	J1
494	CH	NH	1-2	4-Cl, 6-F	Phenyl	J1
495	CH	NH	1-2	4-Cl, 6-F	CF_2CF_3	J1
496	CH	NH	1-2	4-Cl, 6-F	CH_2OCH_3	J1
497	CH	NH	1-2	4-Cl, 6-F	Benzyl	J1
498	CH	NH	1-2	4-Cl, 6-F	4-chlorophenylmethyl	J1
499	CH	NH	1-2	4-Cl, 6-F	SO_2CH_3	J1
500	CH	NH	1-2	4-Cl, 6-F	CF_3	J1
501	CH	NH	1-2	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J1
502	CH	NH	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J1
503	CH	NH	1-2	4-Cl, 6-F	$C(CH_3)_2CH_2OCH_3$	J1
504	CH	NH	1-2	4-Cl, 6-F	C_2H_5	J1
505	CH	NH	1-2	4-Cl, 6-F	CO_2Na	J1
506	CH	NH	1-2	4-Cl, 6-F	$CONHSO_2CH_3$	J1
507	CH	NH	1-2	4-Cl, 6-F	$CHFCH_3$	J1
508	CH	NH	1-2	4-Cl, 6-F	$CH_2CO_2CH_2CH_3$	J1
509	CH	NCH_3	1-2	4-Cl, 6-F	CH_3	J1
510	CH	NCH_3	1-2	4-Cl, 6-F	C_2H_5	J1
511	CH	NCH_3	1-2	4-Cl, 6-F	isopropyl	J1
512	CH	NCH_3	1-2	4-Cl, 6-F	t-butyl	J1
513	CH	NCH_3	1-2	4-Cl, 6-F	CF_3	J1
514	CH	NCH_3	1-2	4-Cl, 6-F	CF_2CF_3	J1
515	CH	NCH_3	1-2	4-Cl, 6-F	$CHFCH_3$	J1
516	CH	NCH_3	1-2	4-Cl, 6-F	$CON(CH_3)_2$	J1
517	CH	NCH_3	1-2	4-Cl, 6-F	$CH_2CO_2C_2H_5$	J1
518	CH	NCH_3	1-2	4-Cl, 6-F	CH_2CH_2CN	J1
519	CH	NCH_3	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J1
520	CH	NCH_3	1-2	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J1
521	CH	NCH_3	1-2	4-Cl, 6-F	$C(CH_3)_2NHSO_2CH_3$	J1
522	CH	NCH_3	1-2	4-Cl, 6-F	$CO_2CH_2CH_3$	J1
523	CH	NC_2H_5	1-2	4-Cl, 6-F	CH_3	J1
524	CH	NC_2H_5	1-2	4-Cl, 6-F	C_2H_5	J1
525	CH	NC_2H_5	1-2	4-Cl, 6-F	isopropyl	J1
526	CH	NC_2H_5	1-2	4-Cl, 6-F	t-butyl	J1
527	CH	NC_2H_5	1-2	4-Cl, 6-F	CF_3	J1
528	CH	NC_2H_5	1-2	4-Cl, 6-F	CO_2CH_3	J1

	529	CH	NC_4H_9	1-2	4-Cl, 6-F	CH_3	J1
	530	CH	NC_4H_9	1-2	4-Cl, 6-F	C_2H_5	J1
	531	CH	NC_4H_9	1-2	4-Cl, 6-F	isopropyl	J1
	532	CH	NC_4H_9	1-2	4-Cl, 6-F	t-butyl	J1
5	533	CH	NC_4H_9	1-2	4-Cl, 6-F	CF_3	J1
	534	CH	NC_4H_9	1-2	4-Cl, 6-F	CO_2CH_3	J1
	535	CH	NCH_2OCH_3	1-2	4-Cl, 6-F	CH_3	J1
	536	CH	NCH_2OCH_3	1-2	4-Cl, 6-F	C_2H_5	J1
	537	CH	NCO_2CH_3	1-2	4-Cl, 6-F	isopropyl	J1
10	538	CH	NCH_2OCH_3	1-2	4-Cl, 6-F	t-butyl	J1
	539	CH	NCH_2OCH_3	1-2	4-Cl, 6-F	CF_3	J1
	540	CH	NCH_2OCH_3	1-2	4-Cl, 6-F	CO_2CH_3	J1
	541	CH	NCO_2CH_3	1-2	4-Cl, 6-F	CH_3	J1
	542	CH	NCO_2CH_3	1-2	4-Cl, 6-F	C_2H_5	J1
15	543	CH	NCO_2CH_3	1-2	4-Cl, 6-F	isopropyl	J1
	544	CH	NCO_2CH_3	1-2	4-Cl, 6-F	t-butyl	J1
	545	CH	NCO_2CH_3	1-2	4-Cl, 6-F	CF_3	J1
	546	CH	NCO_2CH_3	1-2	4-Cl, 6-F	CO_2CH_3	J1
	547	CH	NSO_2CH_3	1-2	4-Cl, 6-F	CH_3	J1
20	548	CH	NSO_2CH_3	1-2	4-Cl, 6-F	C_2H_5	J1
	549	CH	NSO_2CH_3	1-2	4-Cl, 6-F	isopropyl	J1
	550	CH	NSO_2CH_3	1-2	4-Cl, 6-F	t-butyl	J1
	551	CH	NSO_2CH_3	1-2	4-Cl, 6-F	CF_3	J1
	552	CH	NSO_2CH_3	1-2	4-Cl, 6-F	CO_2CH_3	J1
25	553	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	CH_3	J1
	554	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	C_2H_5	J1
	555	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	isopropyl	J1
	556	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	t-butyl	J1
	557	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	CF_3	J1
30	558	CH	NCH_2CHCH_2	1-2	4-Cl, 6-F	CO_2CH_3	J1
	559	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	CH_3	J1
	560	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	C_2H_5	J1
	561	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	isopropyl	J1
	562	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	t-butyl	J1
35	563	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	CF_3	J1
	564	CH	$NCH_2C{\equiv}CH$	1-2	4-Cl, 6-F	CO_2CH_3	J1
	565	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	CH_3	J1
	566	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	C_2H_5	J1
	567	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	isopropyl	J1
40	568	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	t-butyl	J1
	569	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	CF_3	J1
	570	CH	NCH_2CO_2Me	1-2	4-Cl, 6-F	CO_2CH_3	J1
	571	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	CH_3	J1
	572	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	C_2H_5	J1
45	573	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	isopropyl	J1
	574	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	t-butyl	J1
	575	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	CF_3	J1
	576	CH	NCH_2CHF_2	1-2	4-Cl, 6-F	CO_2CH_3	J1
	577	CH	NH	1-2	4-Cl, 6-F	CH_3	J2
50	578	CH	NH	1-2	4-Cl, 6-F	C_2H_5	J2

579	CH	NH	1-2	4-Cl, 6-F	isopropyl	J2
580	CH	NH	1-2	4-Cl, 6-F	t-butyl	J2
581	CH	NH	1-2	4-Cl, 6-F	CF_3	J2
582	CH	NH	1-2	4-Cl, 6-F	CO_2CH_3	J2
583	CH	NH	1-2	4-Cl, 6-F	CH_3	J3
584	CH	NH	1-2	4-Cl, 6-F	C_2H_5	J3
585	CH	NH	1-2	4-Cl, 6-F	isopropyl	J3
586	CH	NH	1-2	4-Cl, 6-F	t-butyl	J3
587	CH	NH	1-2	4-Cl, 6-F	CF_3	J3
588	CH	NH	1-2	4-Cl, 6-F	CO_2CH_3	J3
589	CH	NH	1-2	4-Cl, 6-F	CH_3	J4
590	CH	NH	1-2	4-Cl, 6-F	C_2H_5	J4
591	CH	NH	1-2	4-Cl, 6-F	isopropyl	J4
592	CH	NH	1-2	4-Cl, 6-F	t-butyl	J4
593	CH	NH	1-2	4-Cl, 6-F	CF_3	J4
594	CH	NH	1-2	4-Cl, 6-F	CO_2CH_3	J4
595	CH	NH	1-2	4-Cl	$CO_2CH_2CH_3$	J5
596	CH	NH	1-2	4-Cl, 6-F	CH_3	J5
597	CH	NH	1-2	4-Cl, 6-F	C_2H_3	J5
598	CH	NH	1-2	4-Cl, 6-F	isopropyl	J5
599	CH	NH	1-2	4-Cl, 6-F	t-butyl	J5
600	CH	NH	1-2	4-Cl, 6-F	CF_3	J5
601	CH	NH	1-2	4-Cl, 6-F	CO_2CH_3	J5
602	NH	CH	2-3	4-Cl, 6-F	CH_3	J7
603	NH	CH	2-3	4-Cl, 6-F	n-C_3H_7	J1
604	NH	CH	2-3	4-Cl, 6-F	i-C_3H_7	J1
605	NH	CH	2-3	4-Cl, 6-F	t-C_4H_9	J1
606	NH	CH	2-3	4-Cl, 6-F	CH_2OH	J1
607	NH	CH	2-3	4-Cl, 6-F	CH_2CH_2OH	J1
608	NH	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OH$	J1
609	NH	CH	2-3	4-Cl, 6-F	$CONHCH_3$	J1
610	NH	CH	2-3	4-Cl, 6-F	$CON(CH_3)_2$	J1
611	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J1
612	NH	CH	2-3	4-Cl, 6-F	Phenyl	J1
613	NH	CH	2-3	4-Cl, 6-F	CF_2CF_3	J1
614	NH	CH	2-3	4-Cl, 6-F	CH_2OCH_3	J1
615	NH	CH	2-3	4-Cl, 6-F	Benzyl	J1
616	NH	CH	2-3	4-Cl, 6-F	4-chlorophenylmethyl	J1
617	NH	CH	2-3	4-Cl, 6-F	SO_2CH_3	J1
618	NH	CH	2-3	4-Cl, 6-F	CF_3	J1
619	NH	CH	2-3	4-Cl, 6-F	$C(CH_3)_2OCOCH_3$	J1
620	NH	CH	2-3	4-Cl, 6-F	$C(CH_3)_2CH_2OH$	J1
621	NH	CH	2-3	4-Cl, 6-F	$C(CH_3)_2CH_2OCH_3$	J1
622	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J1
623	NH	CH	2-3	4-Cl, 6-F	CO_2Na	J1
624	NH	CH	2-3	4-Cl, 6-F	$CONHSO_2CH_3$	J1
625	NH	CH	2-3	4-Cl, 6-F	$CHFCH_3$	J1
626	NH	CH	2-3	4-Cl, 6-F	$CH_2CO_2CH_2CH_3$	J1
627	NH	CH	2-3	4-Cl, 6-F	CH_3	J2
628	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J2

629	NH	CH	2-3	4-Cl, 6-F	isopropyl	J2
630	NH	CH	2-3	4-Cl, 6-F	t-butyl	J2
631	NH	CH	2-3	4-Cl, 6-F	CF_3	J2
632	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J2
633	NH	CH	2-3	4-Cl, 6-F	CH_3	J3
634	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J3
635	NH	CH	2-3	4-Cl, 6-F	isopropyl	J3
636	NH	CH	2-3	4-Cl, 6-F	t-butyl	J3
637	NH	CH	2-3	4-Cl, 6-F	CF_3	J3
638	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J3
639	NH	CH	2-3	4-Cl, 6-F	CH_3	J4
640	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J4
641	NH	CH	2-3	4-Cl, 6-F	isopropyl	J4
642	NH	CH	2-3	4-Cl, 6-F	t-butyl	J4
643	NH	CH	2-3	4-Cl, 6-F	CF_3	J4
644	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J4
645	NH	CH	2-3	4-Cl, 6-F	CH_3	J5
646	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J5
647	NH	CH	2-3	4-Cl, 6-F	isopropyl	J5
648	NH	CH	2-3	4-Cl, 6-F	t-butyl	J5
649	NH	CH	2-3	4-Cl, 6-F	CF_3	J5
650	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J5
651	NH	CCH_3	2-3	4-Cl, 6-F	CH_3	J1
652	NH	CCH_3	2-3	4-Cl, 6-F	C_2H_5	J1
653	NH	CCH_3	2-3	4-Cl, 6-F	isopropyl	J1
654	NH	CCH_3	2-3	4-Cl, 6-F	t-butyl	J1
655	NH	CCH_3	2-3	4-Cl, 6-F	CF_3	J1
656	NH	CCH_3	2-3	4-Cl, 6-F	CO_2CH_3	J1
657	NH	CCH_2CH_3	2-3	4-Cl, 6-F	CH_3	J1
658	NH	CCH_2CH_3	2-3	4-Cl, 6-F	C_2H_5	J1
659	NH	CCH_2CH_3	2-3	4-Cl, 6-F	isopropyl	J1
660	NH	CCH_2CH_3	2-3	4-Cl, 6-F	t-butyl	J1
661	NH	CCH_2CH_3	2-3	4-Cl, 6-F	CF_3	J1
662	NH	CCH_2CH_3	2-3	4-Cl, 6-F	CO_2CH_3	J1
663	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	CH_3	J1
664	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	C_2H_5	J1
665	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	isopropyl	J1
666	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	t-butyl	J1
667	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	CF_3	J1
668	NH	CCH_2CHF_2	2-3	4-Cl, 6-F	CO_2CH_3	J1
669	NH	CH	2-3	4-Cl, 6-F	CH_3	J2
670	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J2
671	NH	CH	2-3	4-Cl, 6-F	isopropyl	J2
672	NH	CH	2-3	4-Cl, 6-F	t-butyl	J2
673	NH	CH	2-3	4-Cl, 6-F	CF_3	J2
674	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J2
675	NH	CH	2-3	4-Cl, 6-F	CH_3	J3
676	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J3
677	NH	CH	2-3	4-Cl, 6-F	isopropyl	J3
678	NH	CH	2-3	4-Cl, 6-F	t-butyl	J3

679	NH	CH	2-3	4-Cl, 6-F	CF_3	J3
680	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J3
681	NH	CH	2-3	4-Cl, 6-F	CH_3	J4
682	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J4
683	NH	CH	2-3	4-Cl, 6-F	isopropyl	J4
684	NH	CH	2-3	4-Cl, 6-F	t-butyl	J4
685	NH	CH	2-3	4-Cl, 6-F	CF_3	J4
686	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J4
687	NH	CH	2-3	4-Cl, 6-F	CH_3	J5
688	NH	CH	2-3	4-Cl, 6-F	C_2H_5	J5
689	NH	CH	2-3	4-Cl, 6-F	isopropyl	J5
690	NH	CH	2-3	4-Cl, 6-F	t-butyl	J5
691	NH	CH	2-3	4-Cl, 6-F	CF_3	J5
692	NH	CH	2-3	4-Cl, 6-F	CO_2CH_3	J5
693	NCH_3	CH	2-3	4-Cl, 6-F	CF_3	J1
694	NH	CH	2-3	4-Cl	CF_3	J1
695	CH	NH	1-2	4-Cl, 6-F	CF_3	J1
696	CH	$NCH_2C_6H_5$	1-2	4-Cl, 6-F	CF_3	J1
697	CH	$NCH_2CO_2C_2H_5$	1-2	4-Cl, 6-F	CF_3	J1
698	CH	$NCOCH_3$	1-2	4-Cl, 6-F	CF_3	J1
699	CH	$NCH_2C{\equiv}N$	1-2	4-Cl, 6-F	CF_3	J1
700	CH	NH	1-2	4-Cl, 6-F	CF_3	J1
701	CH	NH	1-2	4-Cl, 6-F	$CO_2C_2H_5$	J1
702	CH	NH	1-2	4-Cl	$CO_2C_2H_5$	J1
703	N	O	1-2	4-Cl, 6-F	CH_3	J7
704	O	CH	1-2	4-Cl, 6-F	$C(CH_3)_2OH$	J7
705	NH	N	2-3	4-Cl, 6-F	CF_3	J6
706	NH	N	2-3	4-Cl, 6-F	$C(CH_3)_3$	J6
707	NH	N	2-3	4-Cl, 6-F	CF_3	J7
708	NH	N	2-3	4-Cl, 6-F	$CH_2C(CH_3)_3$	J1
709	NH	N	2-3	4-Cl, 6-F	3,5-dimethylisoxazolyl	J1
710	NH	N	2-3	4-Cl, 6-F	pyridin-2-yl	J1
711	$NCOCH_3$	N	2-3	4-Cl, 6-F	H	J1
712	NH	N	2-3	4-Cl, 6-F	C_7F_{15}	J1
713	NH	N	2-3	4-Cl, 6-F	$CHCl_2$	J1
714	NH	N	2-3	4-Cl, 6-F	$NHCO_2C_2H_5$	J1
715	NH	N	2-3	4-Cl, 6-F	$CH(CH_3)NHCH_2CO_2C_2H_5$	J1
716	NH	N	2-3	4-Cl, 6-F	$CH(CH_3)OCOCH_3$	J1
717	NH	N	2-3	4-Cl, 6-F	$C(CH_3){=}CH_2$	J1
718	NH	N	2-3	4-Cl, 6-F	$CH{=}C(CH_3)_2$	J1
719	NH	N	2-3	4-Cl, 6-F	$CH(Br)CH_3$	J1
720	NH	N	2-3	6-F	CF_3	J1
721	NH	N	2-3	4-Cl, 6-F	$CH{=}NC_6H_5$	J1
722	NH	N	2-3	4-Cl, 6-F	CH_2OCOCH_3	J1
723	NH	N	2-3	4-Cl, 6-F	$CH(OCH_3)C_6H_5$	J1
724	NH	N	2-3	4-Cl, 6-F	$CH(OCOCH_3)C_6H_5$	J1
725	NH	N	2-3	4-Cl, 6-F	SCH_3	J1
726	NH	N	2-3	4-Cl, 6-F	C_2H_5	J5
727	NCH_3	N	2-3	4,6-Cl_2	CF_3	J1
728	N	NCH_3	2-3	4,6-Cl_2	CF_3	J1

729	NH	NH	----	4-Cl, 6-F	CF_3	J1
730	NH	N	2-3	4,6-Cl_2	CF_3	J5
731	NH	N	2-3	4-Cl, 6-F	SO_2CH_3	J1
732	NH	N	2-3	4-Br,6-F	CF_3	J1
733	NH	N	2-3	4-Br,6-F	C_2H_5	J1
734	NH	N	2-3	4-Cl,6-F	CH_2OH	J1
735	NH	N	2-3	4-Cl,6-F	$C(CH_3)_2OH$	J1
736	NH	N	2-3	4-Cl,6-F	$C(CH_3)OCH_2C_6H_5$	J1
737	NH	N	2-3	4-Cl,6-F	SH	J1
738	NH	N	2-3	4-Cl,6-F	$SCH(CH_3)C{\equiv}N$	J1
739	NH	N	2-3	4-Cl,6-F	SC_2H_5	J1
740	NH	N	2-3	4-Cl,6-F	$SCH_2C{\equiv}CH$	J1
741	NH	N	2-3	4-Cl,6-F	$SCH_2C_6H_5$	J1
742	NH	N	2-3	4-Cl,6-F	$SC{\equiv}N$	J1
743	NH	N	2-3	4-Cl,6-F	$C(CH_3)_2CH_2SC{\equiv}N$	J1
744	NH	N	2-3	4-Cl,6-F	$SCH(CH_3)CO_2C_2H_5$	J1
745	NH	N	2-3	4-Cl,6-F	$SCH(CH_3)CON(CH_3)_2$	J1
746	NH	N	2-3	4-Cl,6-F	$SCH_2C{\equiv}CH$	J5
747	NH	N	2-3	4-Cl,6-F	$SCH_2CH{=}CH_2$	J1
748	NH	N	2-3	4-Cl,6-F	$SCH_2C{\equiv}N$	J1
749	NH	N	2-3	4-Cl,6-F	$SCH_2C{\equiv}CCH_2Cl$	J1
750	O	CH	2-3	4-Cl, 6-F	$CH_2OCONHCH_3$	J1
751	O	CH	2-3	4-Cl, 6-F	$CH_2NHCOCH_2(C_6H_4$, 2-NO_2)	J1
752	O	CH	2-3	4-Cl, 6-F	$C(CH_3)(OH)C_6H_5$	J1
753	O	CH	2-3	4-Cl, 6-F	CH_2NH_2	J1
754	O	CH	2-3	4-Cl, 6-F	$C(CH_3)(OH)CH(CH_3)_2$	J1
755	O	CH	2-3	4-Cl, 6-F	$CH_2NHCOCH_3$	J1
756	O	CH	2-3	4-Cl, 6-F	$CH_2NHSO_2CH_3$	J1
757	O	CH	2-3	4-Cl, 6-F	$C(CH_3)_2F$	J1
758	O	CH	2-3	4-Cl, 6-F	CH_2CO_2H	J1
759	O	CH	2-3	4-Cl, 6-F	$CH_2CON(CH_3)_2$	J1
760	O	CH	2-3	4-Cl, 6-F	$CH_2CON(CH_3)(OCH_3)$	J1
761	O	CH	2-3	4-Cl, 6-F	$CH_2CONHCH_3$	J1
762	O	CH	2-3	4-Cl, 6-F	CH_2CONH_2	J1
763	O	CH	2-3	4-Cl, 6-F	$C_2H_4CON(CH_3)(OCH_3)$	J1
764	O	CH	2-3	4-Cl, 6-F	$C_2H_4CO_2CH_3$	J1
765	O	CH	2-3	4-Cl, 6-F	C_3H_6OH	J1
766	O	CH	2-3	4-Cl, 6-F	$C_2H_4CONHCH_3$	J1
767	NH	N	2-3	4-Cl	SCF_3	J1
768	NH	N	2-3	4-Cl	CF_3	J1
769	NH	N	2-3	4-Cl	CF_3	J3

Table 3 Characterizing Data

Melting Points or Physical States of Representative Compounds

No.	MP/State	No.	MP/State	No.	MP/State	No.	MP/State
1	OIL	246	45-9	377	122-30	722	117-122 RESIN
16	70-72	247	35-8	378	200 C >	723	107-112 RESIN
25	OIL	248	67-71	379	116-22	724	108-114 RESIN
26	OIL	249	84-9	380	201-4	725	135-140 RESIN
28	OIL	250	65-68	381	117-24	726	>210
30	OIL	251	55-7	382	193-5	727	182-183
38	246-9	252	OIL	383	131-40	728	174-175
42	>250	253	GLASS	384	103-5	729	>205
43	SOLID	254	71-5	385	158-160	730	>205
49	OIL	255	134-8	386	132-5	731	150-152 RESIN
96	OIL	256	145-7	387	112-4	732	195-200
98	>245	257	OIL	388	107-9	733	>205
99	OIL	258	232-40	399	177.5-8.5	734	SOLID
100	OIL	259	165-9	405	130	735	118-121 RESIN
101	OIL	260	55-8	469	98-100	736	88-92
102	OIL	261	65-7	481	SOLID	737	>200
103	OIL	262	75-7	493	187-8	738	133-135
104	OIL	263	>50	500	208-10	739	130-132
105	>250	264	155-7	513	178-181	740	178-180
106	OIL	265	130-6	522	78-80	741	118-121 RESIN
107	OIL	266	258-61	527	152-154	742	150-155
108	>250	267	110-8	563	165-166	743	SOLID
109	OIL	268	73-7	595	>240	744	160-162
110	OIL	269	270-5	618	235-237.5	745	>200
112	86-88	270	265-72	693	60-65	746	106-109
221	193.5-6	271	62-72	694	221.5-223	747	98-100
222	183-6	272	OIL	695	160-162	748	104-110 RESIN
223	OIL	273	220-2.5	696	173-177	749	155-158 RESIN
224	OIL	274	116 SOFTENS	697	60-63	750	137-139
225	OIL	275	OIL	698	142-145.5	751	189-190
226	63-6	276	145-53	699	95-102	752	78-82
227	134-6	277	179-82	700	160-162	753	87-89
228	42-5	278	189-92	701	245-248	754	75-77
229	OIL	279	197-8	702	258-260	755	96-98
230	163-5	280	215-6	705	102-103	756	90-92
231	65-70	362	152-8	706	88-89	757	60-62
232	186-91	363	>165	708	140 DEC	758	95-97
233	85-90	364	SOLID	709	>200	759	144-146
234	65-70	365	172-7	710	130 RESIN	760	146-147
235	63-7	366	130	711	>200	761	70-76
236	56-8	367	150-5	712	93-98 RESIN	762	185-187
237	141-2	368	87-93	713	123-130 RESIN	763	63-65
238	143-5	369	125-30	714	160-165 RESIN	764	OIL
239	162-4	370	130	715	90-95	765	50-54
240	72-6	371	SOLID	716	115-120 RESIN	766	172-173
241	67-70	372	SOLID	717	120-125	767	239-241
242	163-5	373	160	718	110-116		
243	51-55	374	190	719	120-125		

No.	MP/State	No.	MP/State	No.	MP/State	No.	MP/State
244	OIL	375	>200	720	128-132 RESIN		
245	OIL	376	142-8	721	145-150		

Biological Testing

The benzofused heterocyclic compounds of this invention were tested for pre- and postemergence herbicidal activity using a variety of crops and weeds. The test plants included soybean (Glycine max var. Winchester), field corn (Zea mays var. Pioneer 3732), wheat (Triticum aestivum var. Lew), morningglory (Ipomea lacunosa or Ipomea hederacea), velvetleaf (Abutilon theophrasti), green foxtail (Setaria viridis), Johnsongrass (Sorghum halepense), blackgrass (Aloepecurus myosuroides), common chickweed (Stellaria media), and common cocklebur (Xanthium strumarium L.).

For preemergence testing, two disposable fiber flats (8 cm x 15 cm x 25 cm) for each rate of application of each candidate herbicide were filled to an approximate depth of 6.5 cm with steam-sterilized sandy loam soil. The soil was leveled and impressed with a template to provide five evenly spaced furrows 13 cm long and 0.5 cm deep in each flat. Seeds of soybean, wheat, corn, green foxtail, and johnsongrass were planted in the furrows of the first flat, and seeds of velvetleaf, morningglory, common chickweed, cocklebur, and blackgrass were planted in the furrows of the second flat. The five-row template was employed to firmly press the seeds into place. A topping soil of equal portions of sand and sandy loam soil was placed uniformly on top of each flat to a depth of approximately 0.5 cm. Flats for postemergence testing were prepared in the same manner except that they were planted 9-14 days prior to the preemergence flats and were placed in a greenhouse and watered, thus allowing the seeds to germinate and the foliage to develop.

In both pre- and postemergence tests, a stock solution of the candidate herbicide was prepared by dissolving 0.27g of the compound in 20 mL of water/acetone (50/50) containing 0.5% v/v sorbitan monolaurate. For an application rate of 3000 g/ha of herbicide a 10 mL portion of the stock solution was diluted with water/acetone (50/50) to 45 mL. The volumes of stock solution and

diluent used to prepare solutions for lower application rates are shown in the following table:

Application Rate (g/ha)	Volume of Stock Solution (mL)	Volume of Acetone/Water (mL)	Total Volume of Spray Solution (mL)
3000	10	35	45
1000	3	42	45
300	1	44	45
100	0.3	45	45.3
30	0.1	45	45.1
10	0.03	45	45.03
3	0.01	45	45.01

The preemergence flats were initially subjected to a light water spray. The four flats were placed two by two along a conveyor belt (i.e., the two preemergence followed by the two postemergence flats). The conveyor belt fed under a spray nozzle mounted about ten inches above the postemergent foliage. The preemergent flats were elevated on the belt so that the soil surface was at the same level below the spray nozzle as the foliage canopy of the postemergent plants. The spray of herbicidal solution was commenced and once stabilized, the flats were passed under the spray at a speed to receive a coverage equivalent of 1000L/ha. At this coverage the application rates are those shown in the above table for the individual herbicidal solutions. The preemergence flats were watered immediately thereafter, placed in the greenhouse and watered regularly at the soil surface. The postemergence flats were immediately placed in the green-house and not watered until 24 hours after treatment with the test solution. Thereafter they were regularly watered at ground level. After 12-17 days the plants were examined and the phytotoxicity data were recorded.

Herbicidal activity data at selected application rates are given for various compounds of this invention in Table 4 and Table 5. The test compounds are identified by numbers which correspond to those in Tables 1 and 2.

Phytotoxicity data were taken as percent control. Percent control was determined by a method similar to the 0 to 100 rating system disclosed in

"Research Methods in Weed Science," 2nd ed., B. Truelove, Ed.; Southern Weed Science Society; Auburn University, Auburn, Alabama, 1977. The rating system is as follows:

Herbicide Rating System

Rating Percent Control	Description of Main Categories	Crop Description	Weed Description
0	No effect	No crop reduction/injury	No weed control
10		Slight discoloration or stunting	Very poor weed control
20	Slight effect	Some discoloration, stunting or stand loss	Poor weed control
30		Crop injury more pronounced but not lasting	Poor to deficient weed control
40		Moderate injury, crop usually recovers	Deficient weed control
50	Moderate effect	Crop injury more lasting, recovery doubtful	Deficient to moderate weed control
60		Lasting crop injury, no recovery	Moderate weed control
70		Heavy injury and stand loss satisfactory	Control somewhat less than
80	Severe	Crop nearly destroyed a few survivors	Satisfactory to weed control
90		Only occasional live plants left	Very good to excellent control
100	Complete effect	Complete crop destruction	Complete weed destruction

Formulation

The compounds of the present invention were tested in the laboratory as water/acetone (50/50) solutions containing 0.5% v/v sorbitan monolaurate

emulsifier. It is expected that all formulations normally employed in applications of herbicides would be usable with the compounds of the present invention. These include wettable powders, emulsifiable concentrates, water suspensions, flowable concentrates, and the like.

Table 4. PREEMERGENCE HERBICIDAL ACTIVITY (% CONTROL)

No.	SOY	WHT	CRN	ABUTH	IPOSS	STEME	XANPE	ALOMY	SETVI	SORHA
1	100	85	90	100	100	100	100	90	100	95
16	100	70	90	100	100	100	90	80	100	95
25	100	100	100	100	100	100	95	90	100	100
26	100	90	90	100	100	100	100	95	100	100
28	100	100	95	100	100	100	100	100	100	100
30	100	100	95	100	100	100	90	100	100	100
38	60	50	80	100	100	0	70	30	75	60
42	0	10	0	100	60	30	20	50	30	0
43	50	40	80	100	100	10	—	60	70	80
49	95	50	80	100	100	20	90	—	100	90
96	100	90	95	100	100	100	—	90	100	95
98	50	40	80	80	75	70	60	10	30	65
99	40	50	60	100	100	100	—	60	100	65
100	40	30	80	100	100	20	—	60	50	70
101	80	70	100	100	100	—	80	80	100	100
102	20	30	10	100	70	—	50	90	100	60
103	50	50	80	100	100	—	70	90	100	70
104	100	100	100	100	100	—	100	100	100	100
106	30	40	70	100	100	95	60	70	90	55
107	80	60	90	100	100	100	40	75	100	100
108	0	0	10	70	50	40	10	50	50	30
109	100	100	90	100	100	100	100	100	100	100
110	100	50	70	100	90	100	40	80	100	100
112	100	100	100	100	100	100	100	100	100	100
221	70	60	85	100	100	80	ND	ND	100	95
222	100	70	90	100	100	100	100	ND	100	100
223	100	50	80	100	100	100	90	ND	100	100
224	100	80	90	100	100	100	95	80	100	100
225	40	20	30	90	50	70	50	ND	100	60
226	70	50	70	100	90	90	60	ND	100	80
227	100	80	90	100	100	100	ND	95	100	100
228	100	80	95	100	100	100	90	ND	100	100
229	100	70	90	100	100	100	95	80	100	100
230	100	40	80	100	100	100	100	80	100	100
231	100	80	100	100	100	100	100	90	100	100
232	20	30	50	90	80	20	10	ND	40	25
233	40	30	70	100	95	20	20	ND	60	50
234	100	100	100	100	100	100	100	80	100	100

	235	100	90	100	100	100	100	100	80	100	100
	236	100	70	95	100	100	100	100	80	100	100
	237	100	90	90	100	100	100	100	100	100	100
	238	100	60	70	100	100	60	80	50	90	90
5	239	100	70	90	100	100	100	ND	ND	100	90
	240	100	95	95	100	100	100	100	ND	100	100
	241	60	70	95	100	100	100	100	ND	100	100
	242	100	100	100	100	100	100	100	100	100	100
	243	100	80	95	100	100	100	100	ND	100	100
10	244	95	80	100	100	90	70	100	70	100	100
	245	100	60	80	100	100	90	100	70	100	80
	246	100	100	100	100	100	100	100	100	100	100
	247	100	90	90	100	100	95	100	85	100	100
	248	100	90	95	100	100	100	100	95	100	100
15	249	100	80	95	100	100	100	90	80	10	100
	250	80	40	50	100	100	ND	100	60	100	70
	251	90	90	95	100	100	95	100	90	100	100
	252	100	100	100	100	100	100	ND	100	100	100
	253	100	95	100	100	100	100	ND	ND	100	100
20	254	25	20	80	100	50	30	50	60	100	80
	255	100	90	95	100	100	100	100	ND	100	100
	256	100	80	95	100	100	100	ND	70	100	90
	257	40	0	10	90	70	0	20	20	70	10
	258	30	30	75	100	60	0	60	ND	40	40
25	259	70	40	80	100	70	100	55	ND	100	95
	260	100	70	80	100	100	100	100	95	100	100
	261	100	80	95	100	100	100	90	80	100	100
	262	90	40	40	100	100	100	100	50	100	70
	263	100	50	65	100	100	100	95	75	100	70
30	264	0	0	10	20	0	20	30	0	10	10
	265	70	40	80	90	100	20	70	ND	80	60
	266	50	30	60	40	70	0	0	ND	30	30
	267	0	10	20	10	10	0	50	50	5	0
	268	30	30	50	100	95	20	0	ND	60	60
35	269	60	30	80	100	100	100	100	70	100	75
	270	70	70	90	100	100	ND	60	65	100	100
	271	80	70	90	100	100	100	100	80	100	90
	272	20	0	20	100	70	100	20	70	90	60
	273	100	80	90	100	100	100	100	90	100	100
40	274	100	100	90	100	100	90	100	95	100	100
	275	100	80	100	100	100	100	100	80	100	95
	362	100	100	100	100	100	100	100	100	100	100
	363	100	100	100	100	100	100	100	100	100	100
	364	100	60	80	100	100	100	100	80	100	80
45	365	ND	30	30	100	100	100	100	60	75	60
	366	10	10	0	70	20	0	10	0	50	40
	367	100	95	100	100	100	100	100	90	100	100
	368	100	100	95	100	100	100	100	95	100	100
	369	100	100	100	100	100	100	100	100	100	100
50	370	100	100	95	100	100	100	100	90	100	100
	371	100	95	100	100	100	100	100	100	100	100
	372	100	90	95	100	100	100	100	80	100	80

373	100	70	90	100	100	100	100	70	100	90
374	30	0	10	100	95	90	80	40	100	75
375	80	30	90	100	80	95	80	80	100	95
376	50	60	80	100	100	100	100	100	100	70
377	100	70	90	100	100	ND	100	100	100	100
378	90	70	90	100	100	100	100	80	100	95
379	100	50	70	100	100	ND	100	80	100	95
380	80	35	20	100	100	ND	80	90	100	70
381	100	40	80	100	100	ND	100	90	100	80
382	60	45	30	100	70	ND	60	90	95	80
383	80	40	20	100	60	ND	70	80	75	55
399	95	80	95	100	95	100	70	60	100	0
493	80	70	90	100	100	100	70	75	100	100
500	95	75	90	100	100	100	100	75	100	100
522	90	40	80	100	100	100	50	75	100	100
595	10	0	0	60	50	10	20	ND	0	40

Rate of Application is 0.3 Kg/Ha. SOY is soybean; WHT is wheat; CRN is corn; ABUTH is velvetleaf; IPOSS is morningglory; STEME is chickweed; XANPE is cocklebur; ALOMY is blackgrass, SETVI is green foxtail; SORHA is johnsongrass

Table 5. POSTEMERGENCE HERBICIDAL ACTIVITY (% CONTROL)

No.	SOY	WHT	CRN	ABUTH	IPOSS	STEME	XANPE	ALOMY	SETVI	SORHA
1	95	65	80	100	100	90	100	70	80	80
16	95	60	80	100	100	70	95	70	80	80
25	100	80	90	100	100	100	100	80	100	90
26	96	60	80	100	100	80	100	80	100	80
28	100	80	80	100	100	100	90	100	100	95
30	95	80	90	100	100	100	100	90	100	100
38	70	35	60	100	100	0	45	20	40	50
42	65	30	60	90	60	—	50	40	100	20
43	80	30	70	100	100	70	50	—	50	50
49	95	70	80	100	100	40	30	—	100	90
96	100	90	90	100	100	100	100	—	100	100
98	40	10	50	60	20	5	20	5	40	20
99	80	40	80	100	100	95	70	—	70	65
100	85	40	60	90	100	50	50	—	30	40
101	95	50	80	100	100	—	—	60	65	65
102	80	30	75	100	100	—	—	60	90	60
103	90	50	80	100	80	—	80	70	100	60
104	100	100	100	100	100	—	—	—	100	100
106	80	30	75	100	100	—	—	60	100	70
107	95	40	100	100	100	100	—	90	100	100
108	50	20	60	20	60	0	10	10	70	20

	109	90	90	80	100	100	—	100	90	100	90
	110	80	40	50	100	100	—	100	70	80	70
	112	100	100	100	100	100	100	100	100	100	100
	221	95	50	60	100	100	100	60	40	70	70
5	222	100	70	90	100	100	100	100	100	100	100
	223	95	40	90	100	100	100	100	ND	100	100
	224	95	70	100	100	100	100	100	90	100	ND
	225	60	30	60	100	75	ND	70	ND	90	60
	226	70	40	80	100	95	80	90	ND	100	80
10	227	95	60	90	100	100	100	100	100	100	100
	228	90	50	80	100	100	80	95	ND	100	90
	229	95	60	80	100	100	100	100	70	100	100
	230	95	40	80	100	100	90	100	70	100	90
	231	100	70	100	100	100	100	ND	100	100	100
15	232	75	50	30	100	80	20	40	ND	30	10
	233	90	30	60	100	100	30	30	ND	30	30
	234	100	100	100	100	100	100	100	100	100	100
	235	100	100	100	100	100	100	100	100	100	100
	236	100	75	90	100	100	100	100	80	100	100
20	237	100	95	100	100	100	ND	100	100	100	100
	238	80	30	70	100	100	ND	100	40	80	70
	239	95	60	80	100	100	100	100	ND	100	80
	240	95	95	100	100	100	100	100	ND	100	100
	241	90	60	70	100	100	85	95	ND	100	70
25	242	100	100	100	100	100	100	100	100	100	100
	243	95	70	95	100	100	100	100	ND	100	100
	244	95	60	90	100	100	100	100	75	100	ND
	245	85	40	75	100	100	60	70	50	70	70
	246	95	100	100	100	100	100	100	ND	100	100
30	247	95	80	100	100	100	100	100	100	100	ND
	248	80	50	95	100	100	100	100	ND	100	100
	249	95	80	100	100	100	100	100	100	100	ND
	250	95	50	80	100	100	80	100	40	100	100
	251	95	70	90	100	100	100	95	100	100	95
35	252	95	90	100	100	100	100	ND	100	100	100
	253	95	100	100	100	100	100	100	ND	100	100
	254	95	40	80	100	70	ND	95	50	100	80
	255	100	100	100	100	100	100	100	ND	100	100
	256	100	80	90	100	100	100	100	80	100	100
40	257	70	20	70	100	60	30	70	30	70	50
	258	80	30	60	80	70	5	50	30	60	50
	259	80	35	75	100	90	30	70	55	80	70
	260	90	80	70	100	100	ND	100	90	100	90
	261	95	80	100	100	100	100	100	100	100	100
45	262	95	60	80	100	100	95	95	50	100	80
	263	95	80	90	100	100	100	100	60	90	70
	264	50	20	50	40	40	0	30	0	ND	20
	265	70	40	60	100	100	30	20	ND	40	20
	266	60	40	60	50	60	10	10	ND	40	40
50	267	50	15	50	80	40	10	10	20	30	20
	268	70	40	60	50	90	20	ND	ND	70	40
	269	90	40	70	100	80	80	ND	ND	70	60

	270	70	40	50	100	60	40	ND	50	50	50
	271	80	40	60	100	100	100	ND	ND	70	50
	272	50	30	45	100	60	50	50	20	70	40
	273	95	60	95	100	100	90	100	80	100	100
5	274	95	60	95	100	100	90	100	90	100	100
	275	100	70	90	100	100	100	100	95	100	100
	362	100	100	100	100	100	100	ND	100	100	100
	363	100	100	100	100	100	ND	100	100	100	100
	364	95	40	80	100	100	100	100	ND	100	100
10	365	100	40	70	100	100	100	ND	70	80	30
	366	70	30	80	95	80	30	100	30	50	50
	367	100	100	100	100	100	100	100	100	100	100
	368	100	100	100	100	100	100	100	100	100	100
	369	100	80	100	100	100	ND	100	100	100	100
15	370	100	95	100	100	100	100	100	100	100	100
	371	95	100	100	100	100	100	100	ND	100	100
	372	100	100	100	100	100	100	100	100	100	100
	373	100	80	100	100	100	100	100	100	100	100
	374	80	25	30	100	95	80	100	25	80	60
20	375	95	40	90	100	95	100	100	90	80	100
	376	90	50	95	100	100	ND	100	90	100	100
	377	95	80	100	100	100	ND	100	100	100	100
	378	90	40	90	100	90	ND	100	80	100	100
	379	95	80	100	100	100	ND	100	70	100	100
25	380	95	30	95	100	100	ND	100	70	100	80
	381	95	40	95	100	100	ND	100	100	100	100
	382	80	40	100	100	100	ND	100	80	90	80
	383	95	40	95	100	95	ND	100	60	95	70
	399	95	30	70	100	100	100	100	50	70	60
30	493	95	60	90	100	100	80	100	65	100	100
	500	95	65	95	100	100	90	100	80	100	100
	522	90	45	90	100	100	100	100	50	100	100
	595	50	10	60	30	40	0	20	10	20	20

35 Rate of Application is 0.3 Kg/Ha. SOY is soybean; WHT is wheat; CRN is corn; ABUTH is velvetleaf; IPOSS is morningglory; STEME is chickweed; XANPE is cocklebur; ALOMY is blackgrass, SETVI is green foxtail; SORHA is johnsongrass

Herbicidal compositions are prepared by combining herbicidally effective amounts of the active compounds with adjuvants and carriers normally employed in the art for facilitating the dispersion of active ingredients for the particular 40 utility desired, recognizing the fact that the formulation and mode of application of a toxicant may affect the activity of the material in a given application. Thus, for agricultural use the present herbicidal compounds may be formulated as granules of relatively large particle size, as water-soluble or water-dispersible granules, as powdery dusts, as wettable powders, as emulsifiable concentrates, as solutions, or

as any of several other known types of formulations, depending on the desired mode of application. It is to be understood that the amounts specified in this specification are intended to be approximate only, as if the word "about" were placed in front of the amounts specified.

These herbicidal compositions may be applied either as water-diluted sprays, or dusts, or granules to the areas in which suppression of vegetation is desired. These formulations may contain as little as 0.1%, 0.2% or 0.5% to as much as 95% or more by weight of active ingredient.

Dusts are free flowing admixtures of the active ingredient with finely divided solids such as talc, natural clays, kieselguhr, flours such as walnut shell and cottonseed flours, and other organic and inorganic solids which act as dispersants and carriers for the toxicant; these finely divided solids have an average particle size of less than about 50 microns. A typical dust formulation useful herein is one containing 1.0 part or less of the herbicidal compound and 99.0 parts of talc.

Wettable powders, also useful formulations for both pre- and post-emergence herbicides, are in the form of finely divided particles which disperse readily in water or other dispersant. The wettable powder is ultimately applied to the soil either as a dry dust or as an emulsion in water or other liquid. Typical carriers for wettable powders include Fuller's earth, kaolin clays, silicas, and other highly absorbent, readily wet inorganic diluents. Wettable powders normally are prepared to contain about 5-80% of active ingredient, depending on the absorbency of the carrier, and usually also contain a small amount of a wetting, dispersing or emulsifying agent to facilitate dispersion. For example, a useful wettable powder formulation contains 80.0 parts of the herbicidal compound, 17.9 parts of Palmetto clay, and 1.0 part of sodium lignosulfonate and 0.3 part of sulfonated aliphatic polyester as wetting agents. Additional wetting agent and/or oil will frequently be added to the tank mix for post-emergence application to facilitate dispersion on the foliage and absorption by the plant.

Other useful formulations for herbicidal applications are emulsifiable concentrates (ECs) which are homogeneous liquid compositions dispersible in water or other dispersant, and may consist entirely of the herbicidal compound and a liquid or solid emulsifying agent, or may also contain a liquid carrier, such as xylene, heavy

aromatic naphthas, isphorone, or other non-volatile organic solvents. For herbicidal application these concentrates are dispersed in water or other liquid carrier and normally applied as a spray to the area to be treated. The percentage by weight of the essential active ingredient may vary according to the manner in which the composition is to be applied, but in general comprises 0.5 to 95% of active ingredient by weight of the herbicidal composition.

Flowable formulations are similar to ECs except that the active ingredient is suspended in a liquid carrier, generally water. Flowables, like ECs, may include a small amount of a surfactant, and will typically contain active ingredients in the range of 0.5 to 95%, frequently from 10 to 50%, by weight of the composition. For application, flowables may be diluted in water or other liquid vehicle, and are normally applied as a spray to the area to be treated.

Typical wetting, dispersing or emulsifying agents used in agricultural formulations include, but are not limited to, the alkyl and alkylaryl sulfonates and sulfates and their sodium salts; alkylaryl polyether alcohols; sulfated higher alcohols; polyethylene oxides; sulfonated animal and vegetable oils; sulfonated petroleum oils; fatty acid esters of polyhydric alcohols and the ethylene oxide addition products of such esters; and the addition product of long-chain mercaptans and ethylene oxide. Many other types of useful surface-active agents are available in commerce. Surface-active agents, when used, normally comprise 1 to 15% by weight of the composition.

Other useful formulations include suspensions of the active ingredient in a relatively non-volatile solvent such as water, corn oil, kerosene, propylene glycol, or other suitable solvents.

Still other useful formulations for herbicidal applications include simple solutions of the active ingredient in a solvent in which it is completely soluble at the desired concentration, such as acetone, alkylated naphthalenes, xylene, or other organic solvents. Granular formulations, wherein the toxicant is carried on relative coarse particles, are of particular utility for aerial distribution or for penetration of cover crop canopy. Pressurized sprays, typically aerosols wherein the active ingredient is dispersed in finely divided form as a result of vaporization of a low boiling dispersant solvent carrier, such as the Freon fluorinated hydrocarbons, may

also be used. Water-soluble or water-dispersible granules are free-flowing, non-dusty, and readily water-soluble or water-miscible. The soluble or dispersible granular formulations described in US 3,920,442 are useful herein with the present herbicidal compounds. In use by the farmer on the field, the granular formulations, emulsifiable concentrates, flowable concentrates, solutions, etc., may be diluted with water to give a concentration of active ingredient in the range of say 0.1% or 0.2% to 1.5% or 2%.

The active herbicidal compounds of this invention may be formulated and/or applied with insecticides, fungicides, nematicides, plant growth regulators, fertilizers, or other agricultural chemicals and may be used as effective soil sterilants as well as selective herbicides in agriculture. In applying an active compound of this invention, whether formulated alone or with other agricultural chemicals, an effective amount and concentration of the active compound is of course employed; the amount may be as low as, e.g. about 1 to 250 g/ha, preferably about 4 to 30 g/ha. For field use, where there are losses of herbicide, higher application rates (e.g., four times the rates mentioned above) may be employed.

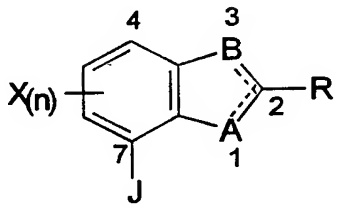
The active herbicidal compounds of the present invention may also be used in combination with other herbicides. Such herbicides include, for example: N-(phosphonomethyl) glycine ("glyphosate"); aryloxyalkanoic acids such as (2,4-dichlorophenoxy)acetic acid ("2,4-D"), (4-chloro-2-methylphenoxy)acetic acid ("MCPA"), (+/-)-2-(4-chloro-2-methylphenoxy)propanoic acid (MCPP); ureas such as N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea ("isoproturon"); imidazolinones such as 2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-3-pyridinecarboxylic acid ("imazapyr"), a reaction product comprising (+/-)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-4-methylbenzoic acid and (+/-)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-5-methylbenzoic acid ("imazamethabenz"), (+/-)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-5-ethyl-3-pyridinecarboxylic acid ("imazethapyr"), and (+/-)-2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-3-quinolinecarboxylic acid ("imazaquin"); diphenyl ethers such as 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid ("acifluorfen"), methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate ("bifenox"), and 5-[2-chloro-4-(trifluoro-

methyl)phenoxy]-N-(methylsulfonyl)-2-nitrobenzamide ("fomasafen"); hydroxybenzonitriles such as 4-hydroxy-3,5-diiodobenzonitrile ("ioxynil") and 3,5-dibromo-4-hydroxybenzonitrile ("bromoxynil"); sulfonylureas such as 2-[[[[(4-chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]benzoic acid ("chlorimuron"), 2-chloro-N-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide ("chlorsulfuron"), 2-[[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]methyl]benzoic acid ("bensulfuron"), 2-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-1-methyl-1H-pyrazol-4-carboxylic acid ("pyrazosulfuron"), 3-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]-2-thiophenecarboxylic acid ("thifensulfuron"), and 2-(2-chloroethoxy)-N-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide ("triasulfuron"); 2-(4-aryloxyphenoxy)alkanoic acids such as (+/-)-2-[4-[(6-chloro-2-benzoxazolyl)oxy]phenoxy]propanoic acid ("fenoxaprop"), (+/-)-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propanoic acid ("fluazifop"), (+/-)-2-[4-(6-chloro-2-quinoxalinyl)oxy]phenoxy]propanoic acid ("quizalofop"), and (+/-)-2-[-(2,4-dichlorophenoxy)phenoxy]propanoic acid ("diclofop"); benzothiadiazinones such as 3-(1-methylethyl)-1H-2,1,3-benzothiadiazin-4(3H)-one 2,2-dioxide ("bentazone"); 2-chloroacetanilides such as N-butoxymethyl)-2-chloro-2',6'-diethylacetanilide ("butachlor"); 2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide ("metachlor"), 2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)acetamide ("acetochlor"), and (RS)-2-chloro-N-(ethoxymethyl)-N-(2-methoxy-1-methylethyl)acetamide ("dimethenamide"); arenecarboxylic acids such as 3,6-dichloro-2-methoxybenzoic acid ("dicamba"); and pyridyloxyacetic acids such as [(4-amino-3,5-dichloro-6-fluoro-2-pyridinyl)oxy]acetic acid ("fluroxypyr").

It is apparent that various modifications may be made in the formulations and application of the compounds of the present invention without departing from the inventive concepts herein, as defined in the claims.

We claim:

1. A compound having the formula



where

(1) A is nitrogen double-bonded to position 2 and B is oxygen;

(2) A is oxygen and B is CR^1 double bonded to position 2;

(3) A is NH and B is nitrogen double-bonded to position 2;

(4) A is nitrogen double bonded to position 2 and B is NR^2;

(5) A is CH double bonded to position 2 and B is NR^2;

(6) A is NH and B is CR^1 double bonded to position 2; or

(7) A and B are NH;

R is hydrogen, hydroxy, mercapto, straight or branched chain lower alkyl, cycloalkyl, alkoxy, aryl, heteroaryl, alkenyl, haloalkyl, hydroxyalkyl, haloaryl, alkoxyaryl, arylalkyl, aryloxyalkyl, haloarylalkyl, alkylthio, heterocyclyl, alkoxyalkyl, alkoxylalkyloxyalkyl, alkylcarbonyloxyalkyl, arylcarbonyloxyalkyl, aminocarbonyloxyalkyl, aminoalkyl, cyanoalkyl, aminoalkenyl, carboxy, carboxyalkyl, alkylcarboxy, alkylcarboxyalkyl, formyl, aminocarbonyl, amino, oxygen, cyano, nitro, alkylsulfonyl, aminosulfonyl, alkylsulfonylamino, alkylcarboxyoxyalkyl, akylcarboxylalkoxy, alkoxycarbonylamino, alkoxycarbonylalkylaminoalkyl, aryliminoalkyl, (aryl)(alkoxy)alkyl, (aryl)(alkylcarbonyloxy)alkyl, arylalkoxyalkyl, cyanoalkylthio, alkynylalkylthio, arylalkylthio, cyanothio, cyanothioalkyl, alkoxycarbonylalkylthio, aminocarbonylalkylthio, alkenylalkylthio, haloalkylalkynylalkylthio, aminocarbonyloxyalkyl, arylalkylcarbonylaminoalkyl, (hydroxy)(aryl)alkyl, alkylcarbonylaminoalkyl, alkylsulfonylaminoalkyl, aminocarbonylalkyl, alkoxycarbonyl, and alkenyloxy, where the amino group may be substituted with one or two substituents independently selected from alkyl, hydroxy, alkoxy, carboxy, aryl, alkylsufonyl or haloalkylsulfonyl;

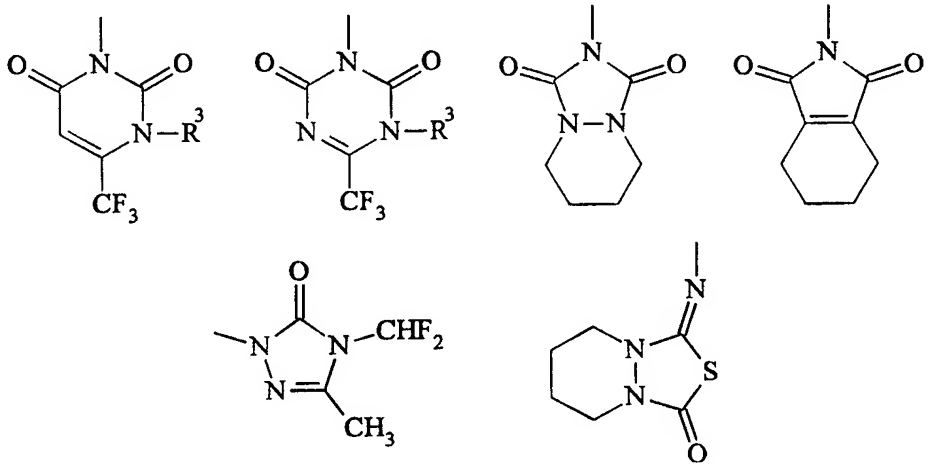
R^1 is hydrogen, lower alkyl, or haloalkyl;

R^2 is hydrogen, alkyl, haloalkyl, CO_2(alkyl), CH_2CO_2(alkyl), CH_2CONH(alkyl), CH_2CON(alkyl)$_2$, CH_2CO_2H, CH_2OCH_3, SO_2(alkyl), $CH_2CH=CH_2$, or $CH_2C\equiv CH$;

X is selected from hydrogen, F, Cl, Br, alkyl, haloalkyl, CN, NO_2, and NH_2;

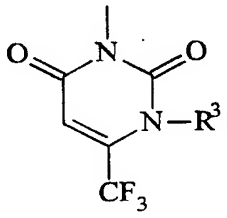
n is 0-3;

J is selected from



and R^3 is selected from hydrogen, alkyl, haloalkyl, CH_2CN, $CH_2CH=CH_2$, $CH_2C\equiv CH$, CH_2CO_2(alkyl), CH_2OCH_3, and NH_2;

with the proviso that J is not



when:

A is oxygen and B is CR^1 double bonded to position 2;

A is CH double bonded to position 2 and B is NR^2; or

A is NH and B is CR^1 double bonded to position 2.

2. A compound of claim 1 in which A is nitrogen double-bonded to position 2 and B is oxygen.

3. A compound of claim 1 in which A is oxygen and B is CR^1 double bonded to position 2.

4. A compound of claim 1 in which A is NH and B is nitrogen double-bonded to position 2.

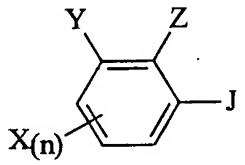
5. A compound of claim 1 in which A is nitrogen double bonded to position 2 and B is NR^2.

6. A compound of claim 1 in which A is CH double bonded to position 2 and B is NR^2.

7. A compound of claim 1 in which A is NH and B is CR^1 double bonded to position 2.

8. A compound of claim 1 in which A and B are NH.

9. A compound having the formula



where X is selected from hydrogen, F, Cl, Br, alkyl, haloalkyl, CN, NO_2, and NH_2;

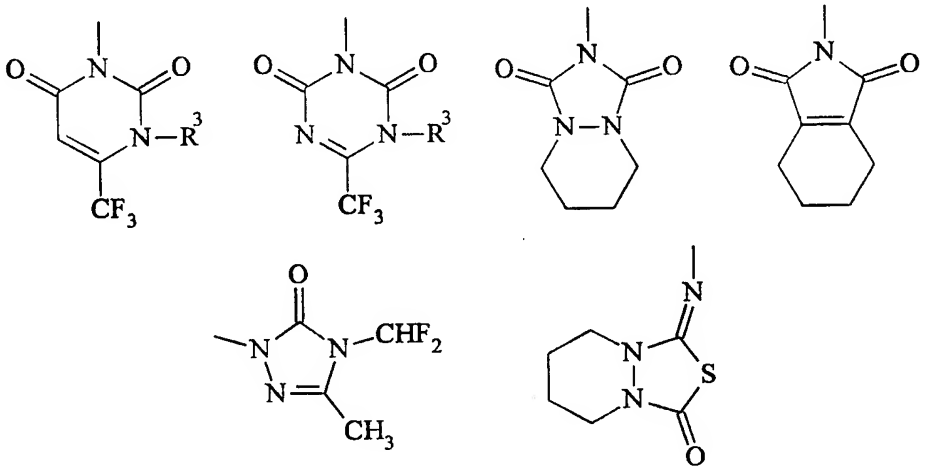
Y is selected from NO_2, NH_2, or -NHN=C(CH_3)R;

Z is selected from hydrogen, F, NH_2, OH; with the proviso that when Y is -NHN=C(CH_3)R, Z is hydrogen;

n is 0-3;

R is hydrogen, hydroxy, straight or branched chain lower alkyl, cycloalkyl, alkoxy, aryl, heteroaryl, alkenyl, haloalkyl, hydroxyalkyl, haloaryl, alkoxyaryl, arylalkyl, aryloxyalkyl, haloarylalkyl, alkylthio, heterocyclyl, alkoxyalkyl, alkoxylalkyloxyalkyl, alkylcarbonyloxyalkyl, arylcarbonyloxyalkyl, aminocarbonyloxyalkyl, aminoalkyl, cyanoalkyl, aminoalkenyl, carboxy, carboxyalkyl, alkylcarboxy, alkylcarboxyalkyl, formyl, aminocarbonyl, amino, oxygen, cyano, nitro, alkylsulfonyl, alkylcarboxyoxyalkyl, akylcarboxylalkoxy, alkoxycarbonylamino, alkoxycarbonylalkylaminoalkyl, aryliminoalkyl, (aryl)(alkoxy)alkyl, (aryl)(alkylcarbonyloxy)alkyl, arylalkoxyalkyl, cyanoalkylthio, alkynylalkylthio, arylalkylthio, cyanothio, cyanothioalkyl, alkoxycarbonylalkylthio, aminocarbonylalkylthio, alkenylalkylthio, haloalkylalkynylalkylthio, aminocarbonyloxyalkyl, arylalkylcarbonylaminoalkyl, (hydroxy)(aryl)alkyl, alkylcarbonylaminoalkyl, alkylsulfonylaminoalkyl, aminocarbonylalkyl, alkoxycarbonyl, and alkenyloxy, where the amino group may be substituted with one or two substituents independently selected from alkyl, hydroxy, alkoxy, carboxy, aryl, or alkylsufonyl;

J is selected from



and R^3 is selected from hydrogen, alkyl, haloalkyl, CH_2CN, $CH_2CH=CH_2$, $CH_2C\equiv CH$, CH_2CO_2(alkyl), CH_2OCH_3, and NH_2.

10. An herbicidal composition comprising an herbicidally effective amount of a compound of claim 1, and an herbicidally compatible carrier therefor.

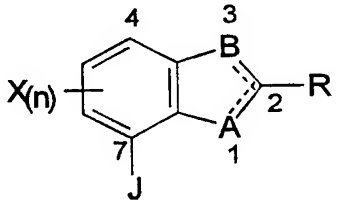
11. An herbicidal composition comprising an herbicidally effective amount of a compound of claim 1 and an herbicidally effective amount of one or more herbicides selected from the group consisting of glyphosate, 2,4-D, MCPA, MCPP, isoproturon, imazapyr, imazamethabenz, imazethapyr, imazaquin, acifluorfen, bifenox, fomasafen, ioxynil, bromoxynil, chlorimuron, chlorsulfuron, bensulfuron, pyrazosulfuron, thifensulfuron, triasulfuron, fenoxaprop, fluazifop, quizalofop, diclofop, bentazone, butachlor, metachlor, acetochlor, dimethenamide, dicamba, and fluroxypyr.

12. An herbicidal composition comprising an herbicidally effective amount of a compound of claim 1, and an herbicidally compatible carrier therefor.

13. A method of controlling undesired plant growth, comprising application to the locus where the undesired plants are growing or are expected to grow, an herbicidally effective amount of a composition of claim 1.

14. A method of controlling undesired plant growth, comprising application to the locus where the undesired plants are growing or are expected to grow, an herbicidally effective amount of a composition of claim 11.

15. A compound having the formula



where

A is oxygen and B is CR^1 double bonded to position 2;

A is CH double bonded to position 2 and B is NR^2; or

A is NH and B is CR^1 double bonded to position 2;

R is hydrogen, hydroxy, mercapto, straight or branched chain lower alkyl, cycloalkyl, alkoxy, aryl, heteroaryl, alkenyl, haloalkyl, hydroxyalkyl, haloaryl, alkoxyaryl, arylalkyl, aryloxyalkyl, haloarylalkyl, alkylthio, heterocyclyl, alkoxyalkyl, alkoxylalkyloxyalkyl, alkylcarbonyloxyalkyl, arylcarbonyloxyalkyl, aminocarbonyloxyalkyl, aminoalkyl, cyanoalkyl, aminoalkenyl, carboxy, carboxyalkyl, alkylcarboxy, alkylcarboxyalkyl, formyl, aminocarbonyl, amino, oxygen, cyano, nitro, alkylsulfonyl, aminosulfonyl, alkylsulfonylamino, alkylcarboxyoxyalkyl, akylcarboxylalkoxy, alkoxycarbonylamino, alkoxycarbonylalkylaminoalkyl, aryliminoalkyl, (aryl)(alkoxy)alkyl, (aryl)(alkylcarbonyloxy)alkyl, arylalkoxyalkyl, cyanoalkylthio, alkynylalkylthio, arylalkylthio, cyanothio, cyanothioalkyl, alkoxycarbonylalkylthio, aminocarbonylalkylthio, alkenylalkylthio, haloalkylalkynylalkylthio, aminocarbonyloxyalkyl, arylalkylcarbonylaminoalkyl, (hydroxy)(aryl)alkyl, alkylcarbonylaminoalkyl, alkylsulfonylaminoalkyl, aminocarbonylalkyl, alkoxycarbonyl, and alkenyloxy, where the amino group may be substituted with one or two substituents independently selected from alkyl, hydroxy, alkoxy, carboxy, aryl, alkylsufonyl or haloalkylsulfonyl;

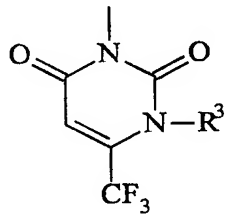
R^1 is hydrogen, lower alkyl, or haloalkyl;

R^2 is hydrogen, alkyl, haloalkyl, CO_2(alkyl), CH_2CO_2(alkyl), CH_2CONH(alkyl), $CH_2CON(alkyl)_2$, CH_2CO_2H, CH_2OCH_3, SO_2(alkyl), $CH_2CH{=}CH_2$, or $CH_2C{\equiv}CH$;

X is selected from hydrogen, F, Cl, Br, alkyl, haloalkyl, CN, NO_2, and NH_2;

n is 0-3;

J is



and R^3 is selected from hydrogen, alkyl, haloalkyl, CH_2CN, $CH_2CH{=}CH_2$, $CH_2C{\equiv}CH$, CH_2CO_2(alkyl), CH_2OCH_3, and NH_2.

INTERNATIONAL SEARCH REPORT

In: tional Application No
PCT/US 98/03647

A. CLASSIFICATION OF SUBJECT MATTER
IPC 6 C07D405/04 C07D403/04 A01N43/54 C07D413/04 C07D209/48
C07D487/04 C07D513/04 C07D239/54 C07D251/16 C07D249/08
A01N43/76 A01N43/66 A01N43/653 A01N43/52

According to International Patent Classification(IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 6 C07D A01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	EP 0 617 033 A (SUMITOMO CHEMICAL CO) 28 September 1994 see claims ---	1-8, 10-15
Y	EP 0 561 319 A (SUMITOMO CHEMICAL CO) 22 September 1993 see claims ---	1-8, 10-15
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Y	WO 95 05079 A (FMC CORP) 23 February 1995 see claims --- -/--	1-8, 10-15

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

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"A" document defining the general state of the art which is not considered to be of particular relevance

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"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

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"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
12 June 1998	23/06/1998

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Henry, J

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INTERNATIONAL SEARCH REPORT

Int tional Application No
PCT/US 98/03647

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

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X	EP 0 255 047 A (HOFFMANN LA ROCHE) 3 February 1988 see claims 21,22	9
X	DE 195 23 640 A (BAYER AG) 2 January 1997 see page 11; examples II-3	9
X	DE 195 04 188 A (BASF AG) 14 August 1996 see page 27	9
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